Generative Models for Hadronic Shower Simulation

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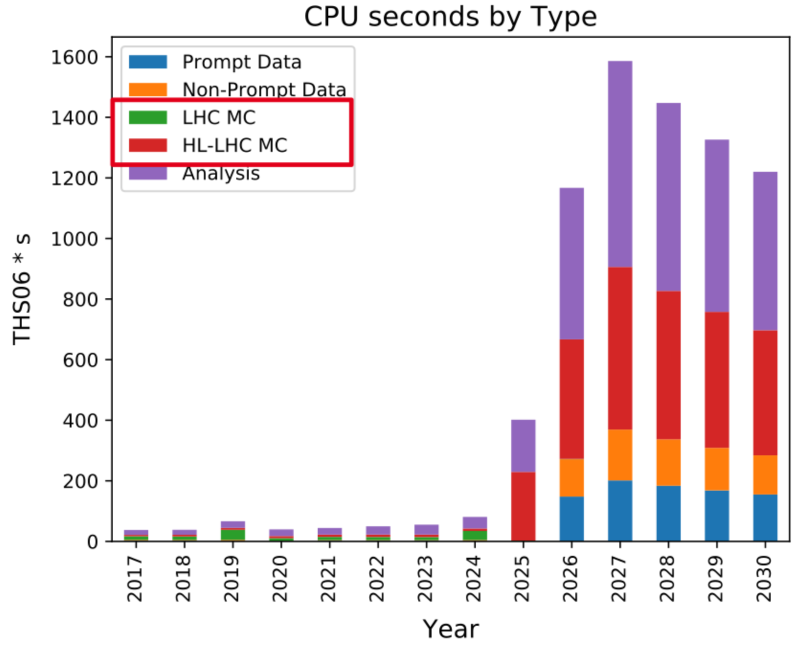
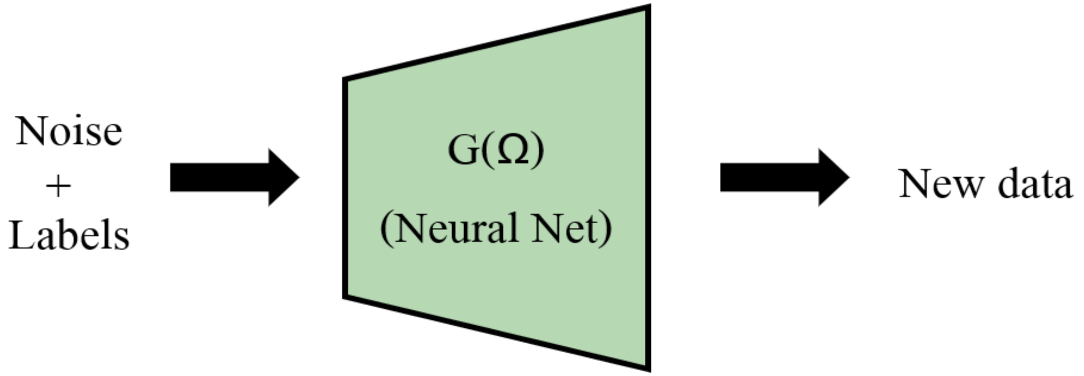
5th Inter Experiment Machine Learning Workshop

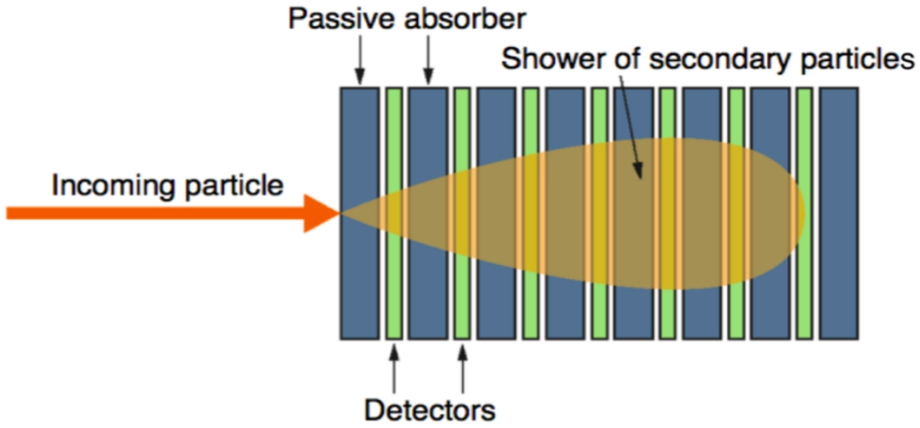
The bottleneck in HEP Computing Resources

- MC simulation is computationally intensive
  - Calorimeters most intensive part of detector simulation
- **Generative models** potentially offer orders of magnitude speed up
- Amplify statistics of original data set
  - Generate new samples following distribution of original data
  - Significant less time per shower

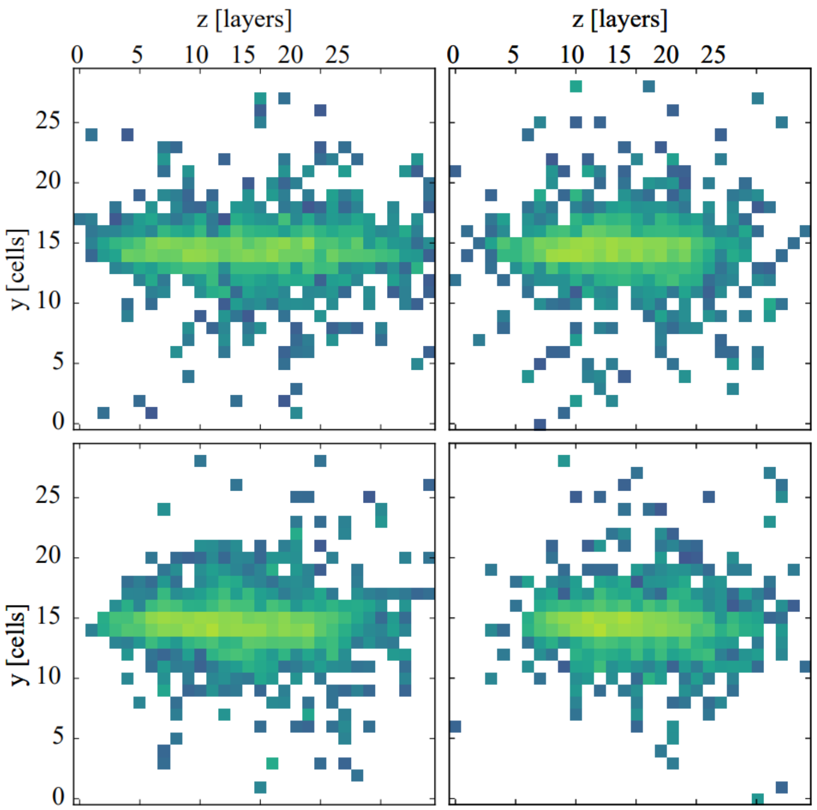


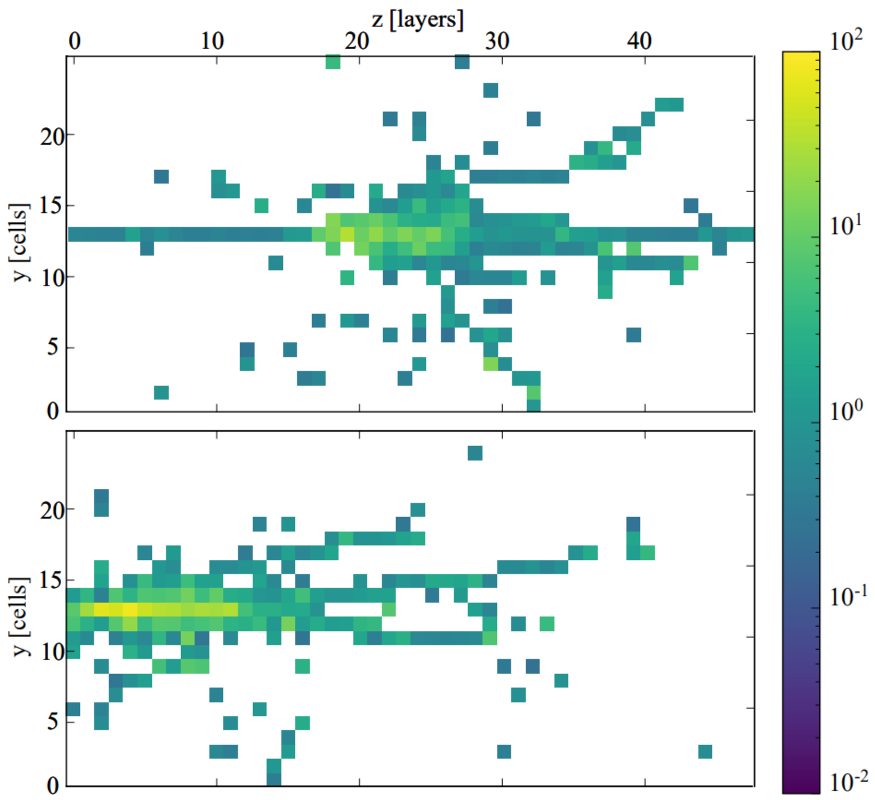
The HEP Software Foundation., Albrecht, J., Alves, A.A. et al. A Roadmap for HEP Software and Computing R&D for the 2020s. Comput Softw Big Sci 3, 7 (2019).





From Photons to Pions





Photon showers

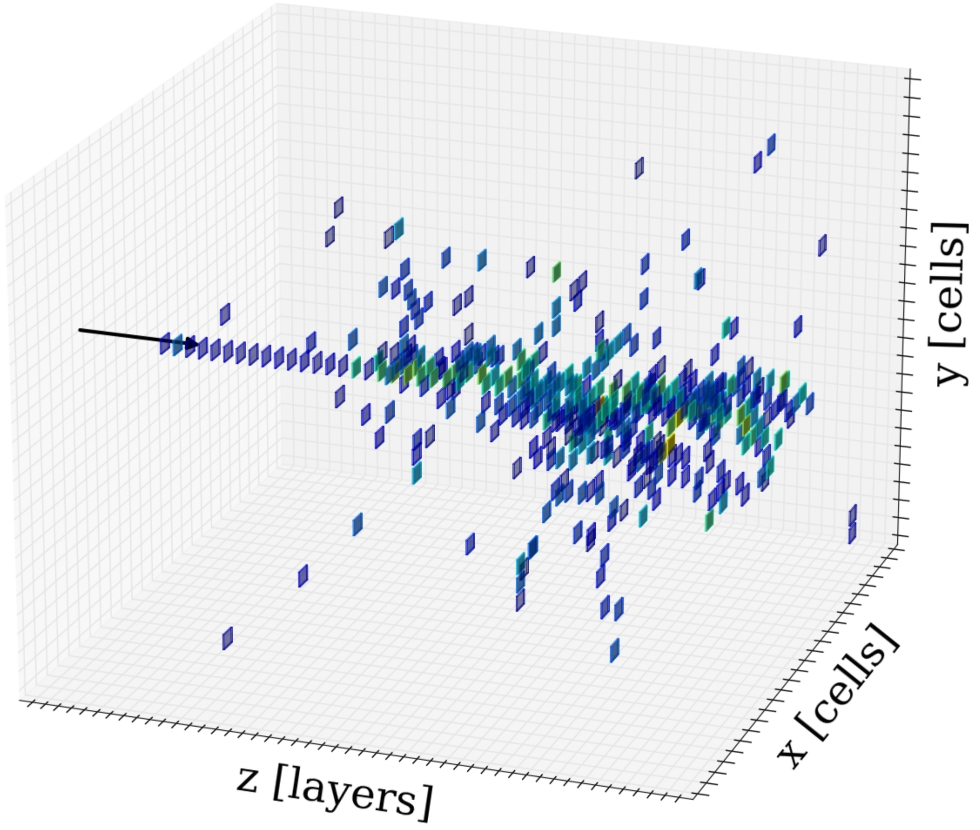
- Predominantly governed by EM interactions
- Compact structure → **Easy to generalise**

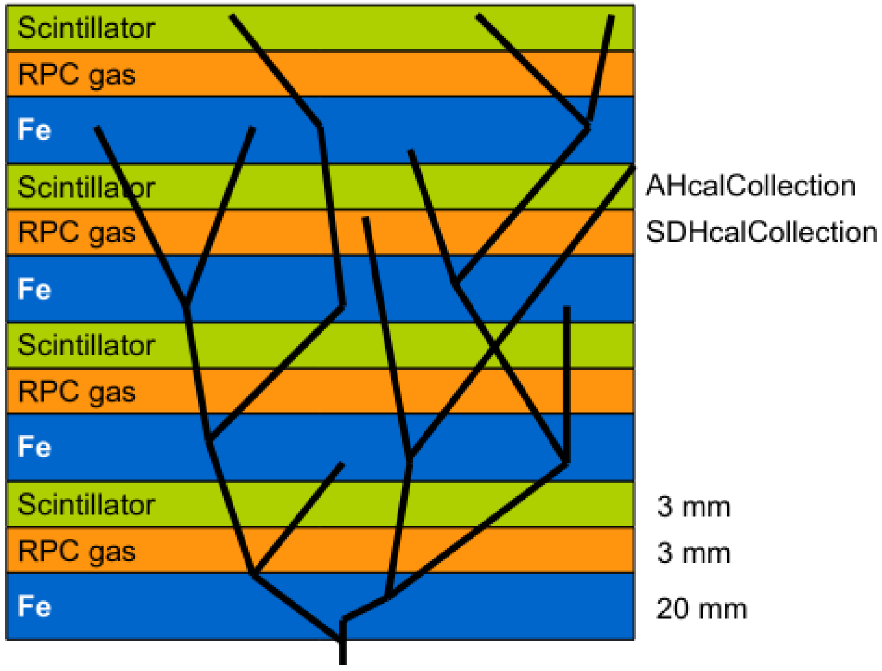
Pion showers

- Hadronic and EM interactions
- Complex structure
- Large event-to-event fluctuations

→ **Hard to learn**

Pion Dataset





- 500k showers generated with Geant4
- Fixed incident point and angle
- Projected onto **48 x 25 x 25**
- Uniform energy: 10 GeV to 100 GeV

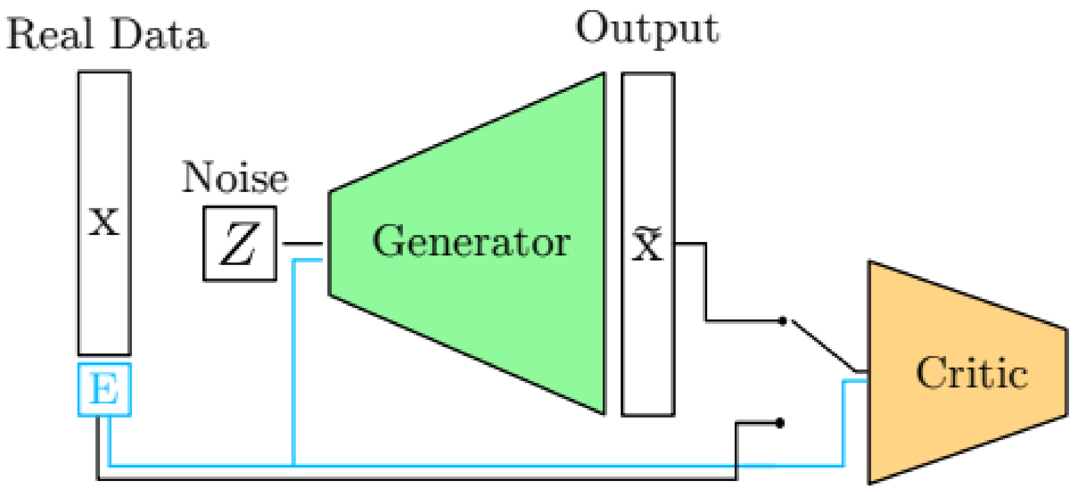
Hybrid simulation of ILD Hadron Calorimeter:

- Hits are recorded for scintillator and RPCs at the same time
- Here only scintillator option is used

Architectures: GAN and WGAN

Generative Adversarial Neural Network

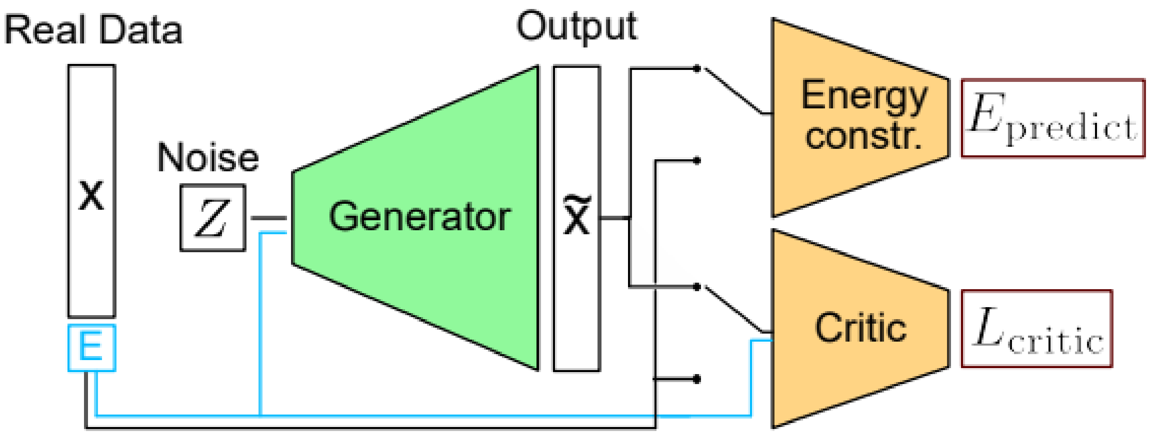
- Original generative architecture applied for shower generation
- Discriminator and Generator play a min-max game



Wasserstein GAN

- Alternative to classical GAN training
- Wasserstein-1 distance as loss with gradient penalty: **improve stability**

- **Addition of an auxiliary constrainer networks for improved conditioning performance**



$$L = L_{\text{critic}} + |E_{\text{predicted}} - E_{\text{label}}|$$

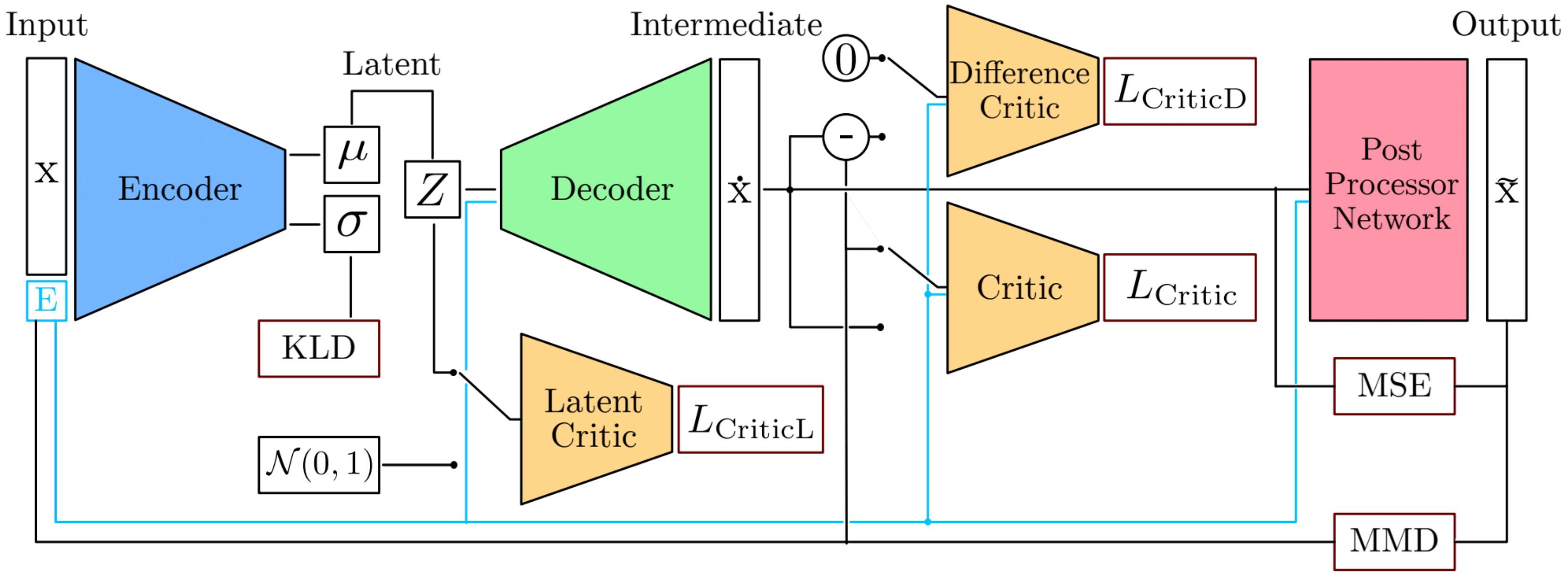
Architectures: BIB-AE

Bounded-Information Bottleneck Autoencoder (BIB-AE)

[*] Voloshynovskiy et. al: **Information bottleneck through variational glasses**, arXiv:1912.00830

[**] Buhmann et. al: **Decoding Photons: Physics in the latent space of a BIB-AE Generative Network**, arXiv:2102.12491

- Unifies features of both GANs and Variational Autoencoders [*]
- Post-Processor network: Improve per-pixel energies; second training
- Multi-dimensional KDE sampling: better modeling of latent space [**]

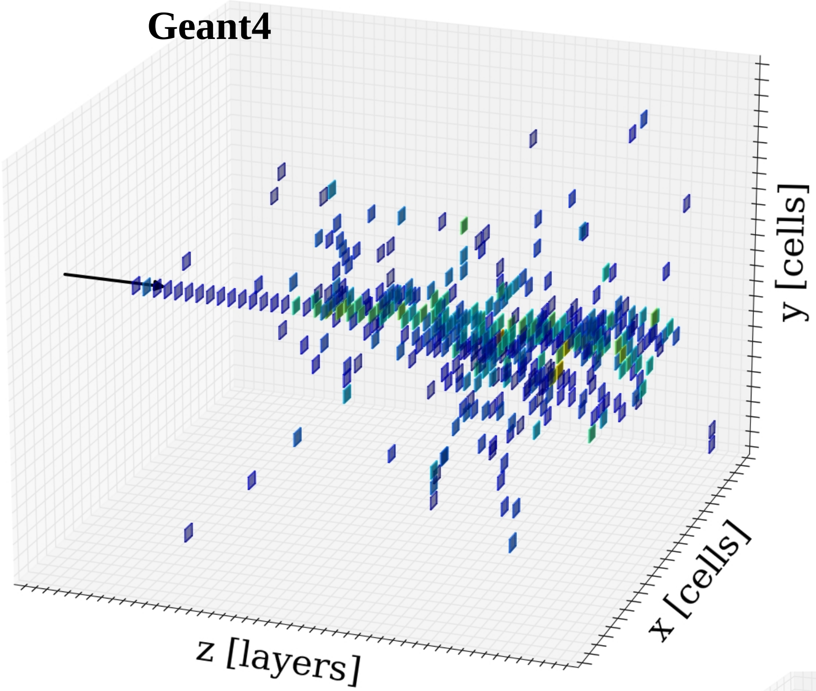


$$L_{\mathrm{BIB-AE}} = \mathrm{KLD} + L_{\mathrm{CriticL}} + L_{\mathrm{Critic}} + L_{\mathrm{CriticD}}$$

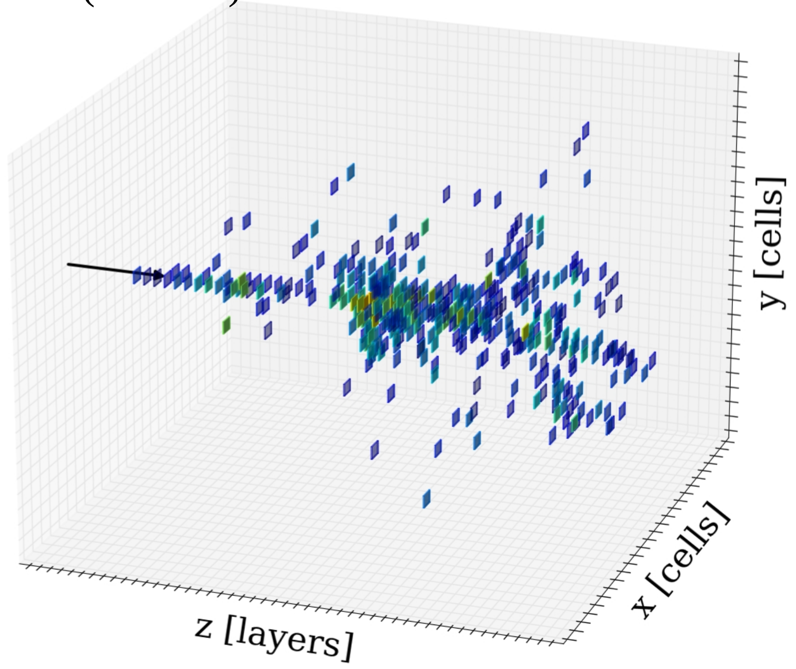
$$L_{\mathrm{Post}} = \mathrm{MMD} + \mathrm{MSE}$$

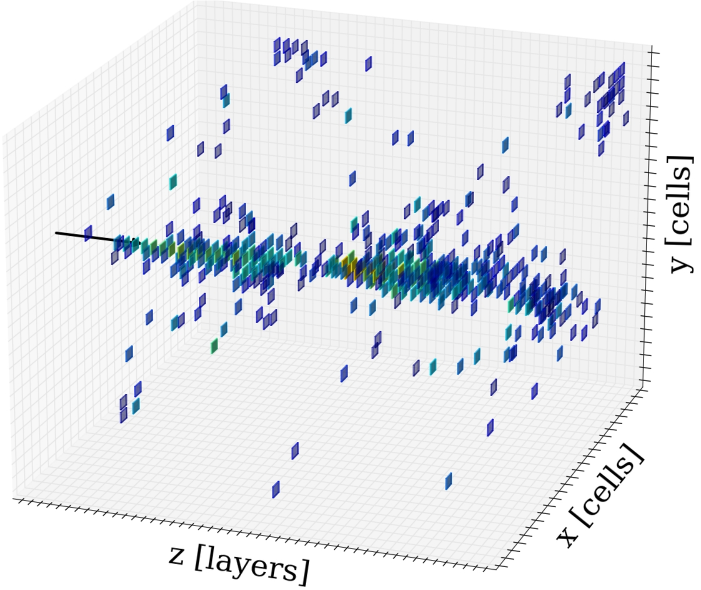
Visual Inspection

At first glance



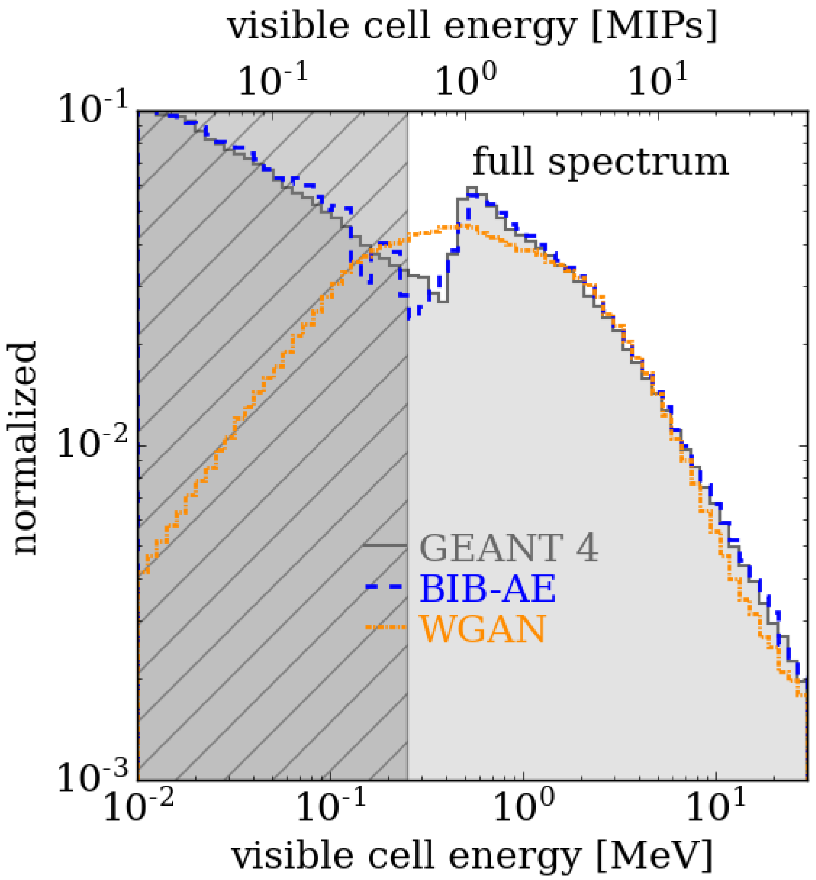
Synthetic Shower
(BIB-AE)

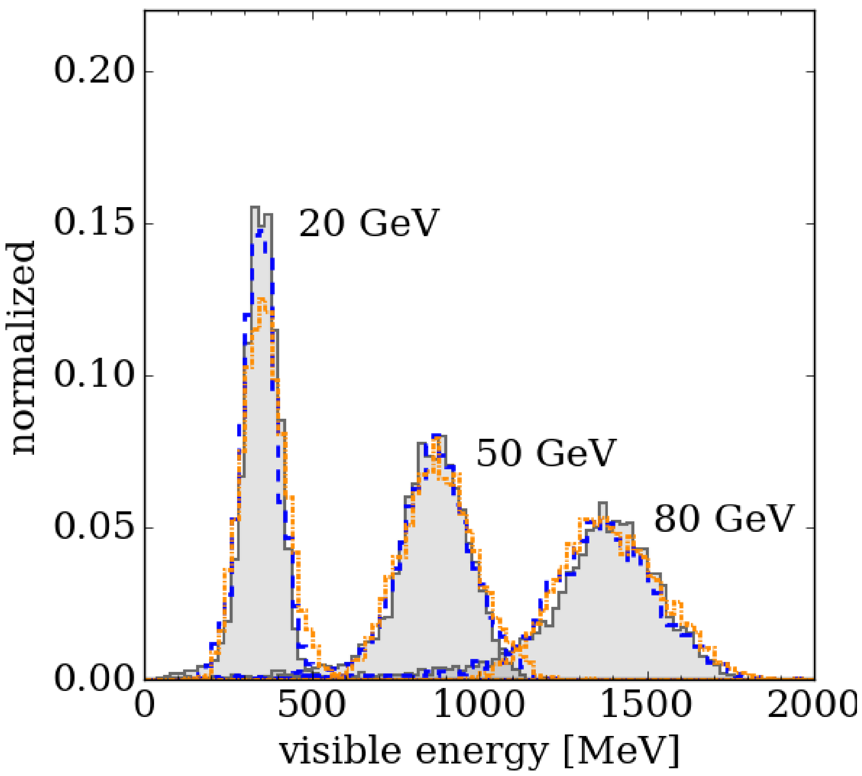


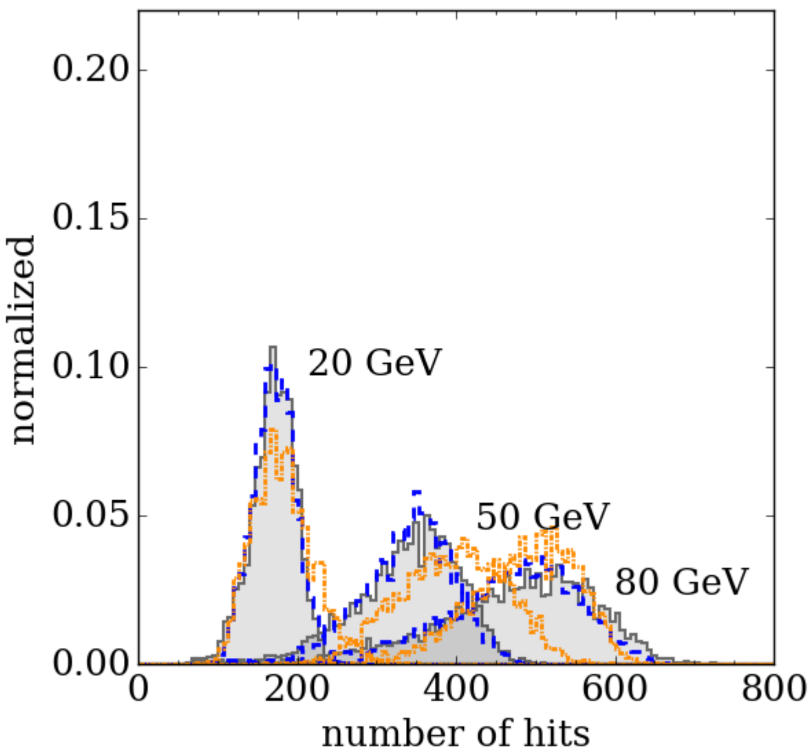


Synthetic Shower
(WGAN)

Pion Shower Results I







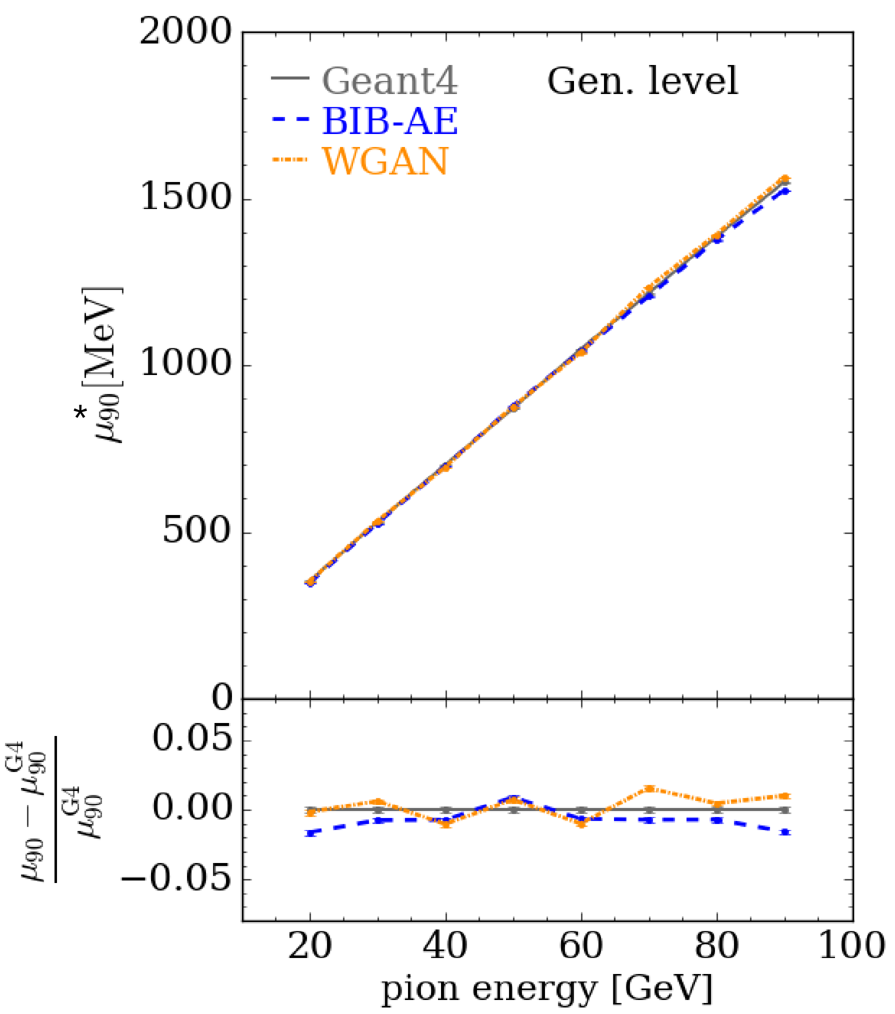
Very good agreement of MIP peak for **BIB-AE** with Post-Processing!

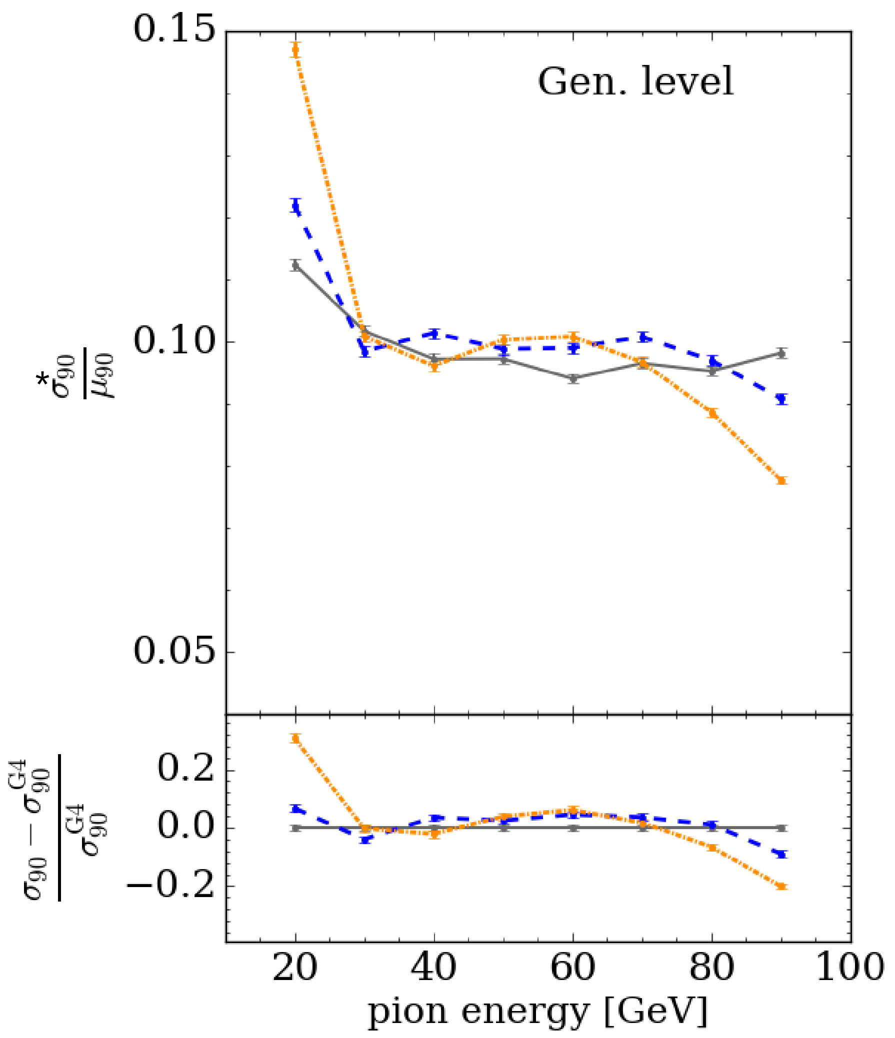
Great agreement with Geant4

Too much hits for **WGAN** ~50 GeV
BIB-AE is better

arXiv:2112.09709

Pion Shower Results II

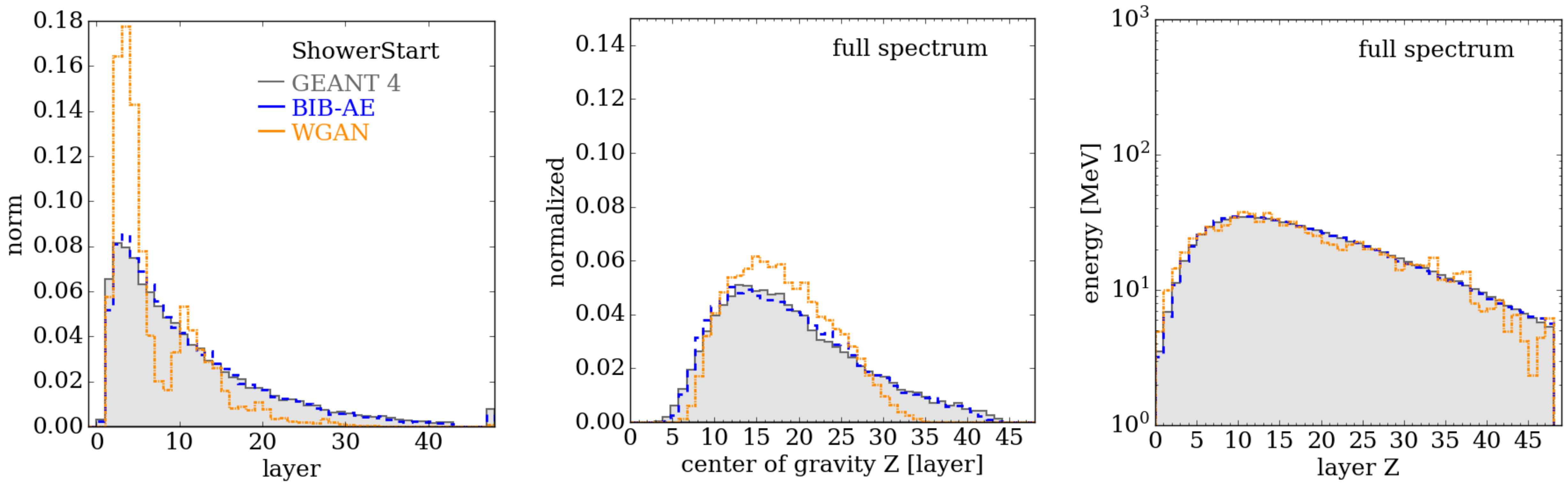




Very crucial quantity to get it right

*the mean and root-mean-square of the 90% core of visible energy distributions

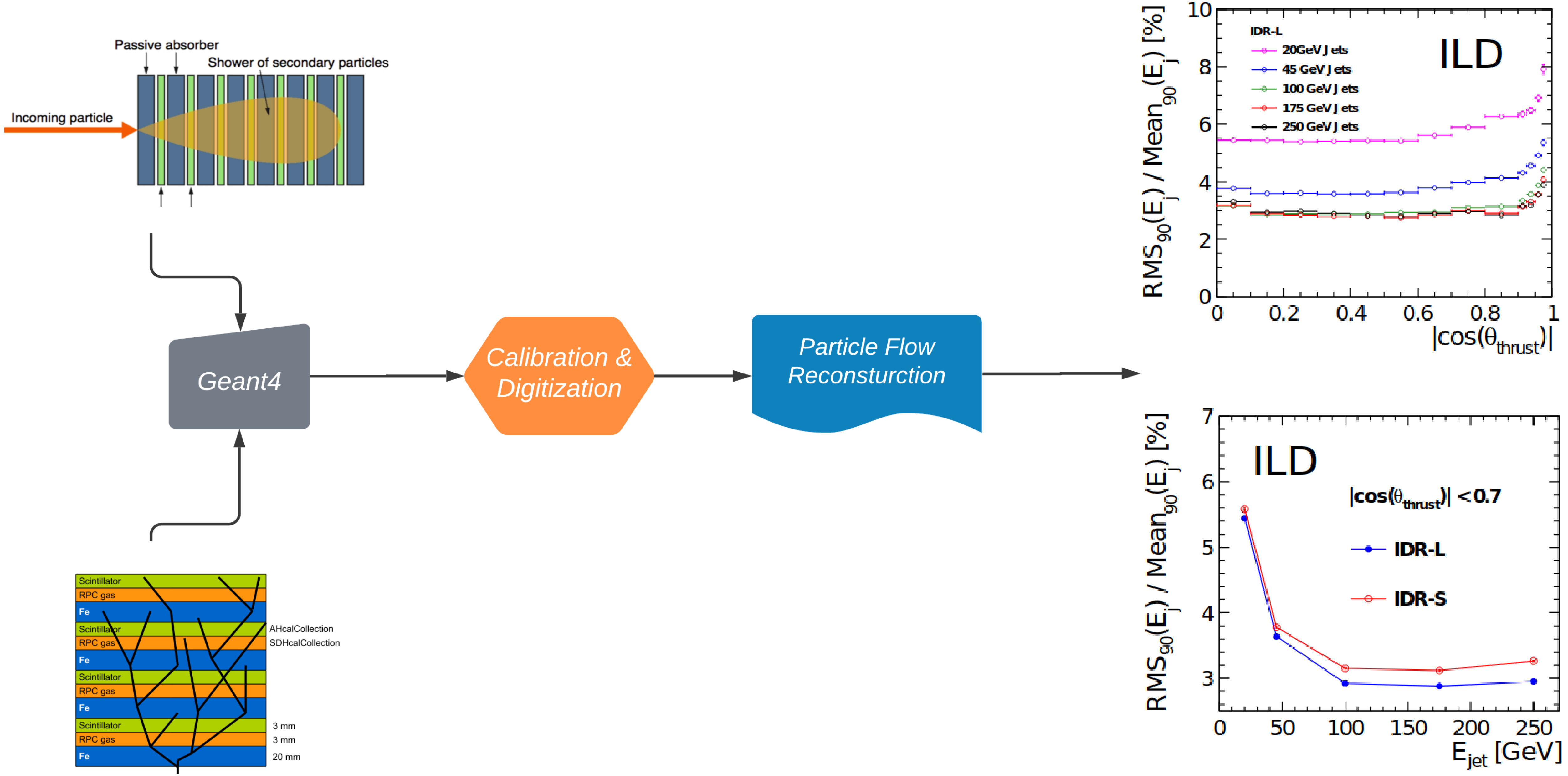
Pion Shower Results III



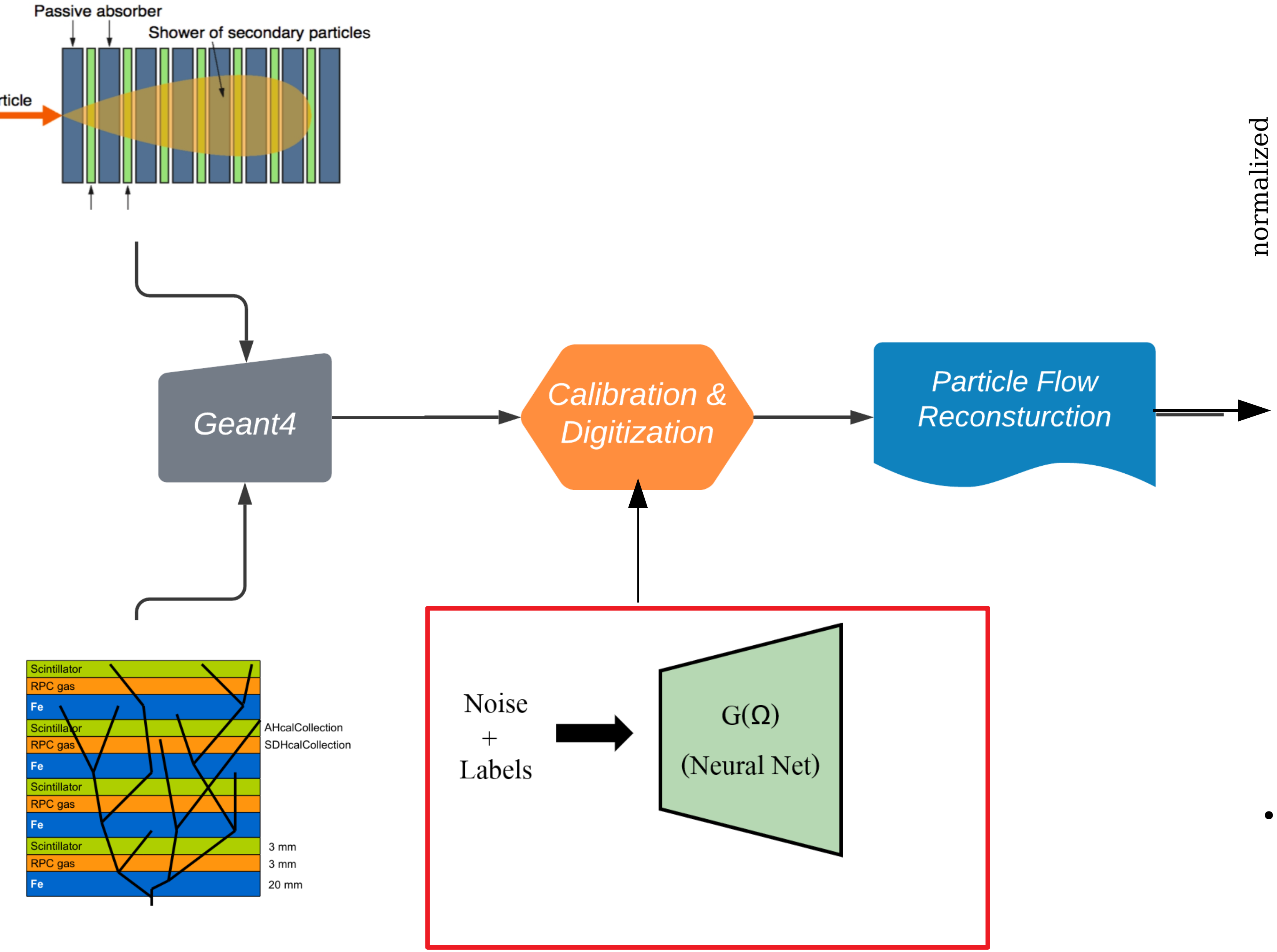
BIB-AE reproduces Geant4 distributions

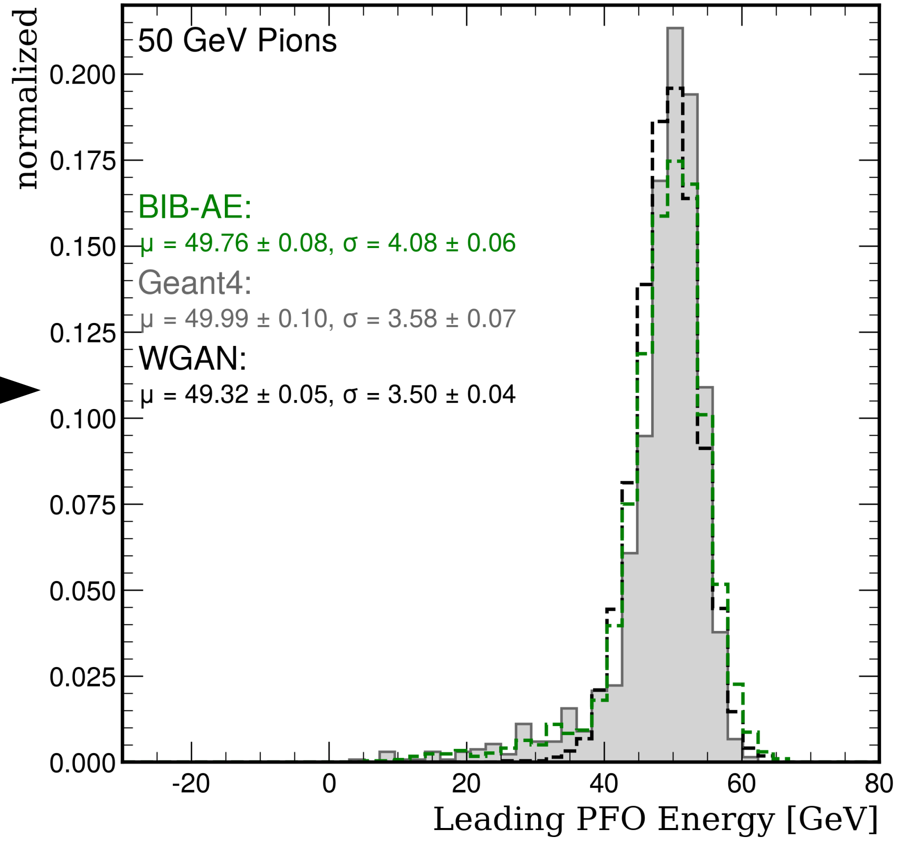
WGAN performance is not as great...

ILD Analysis Pipeline



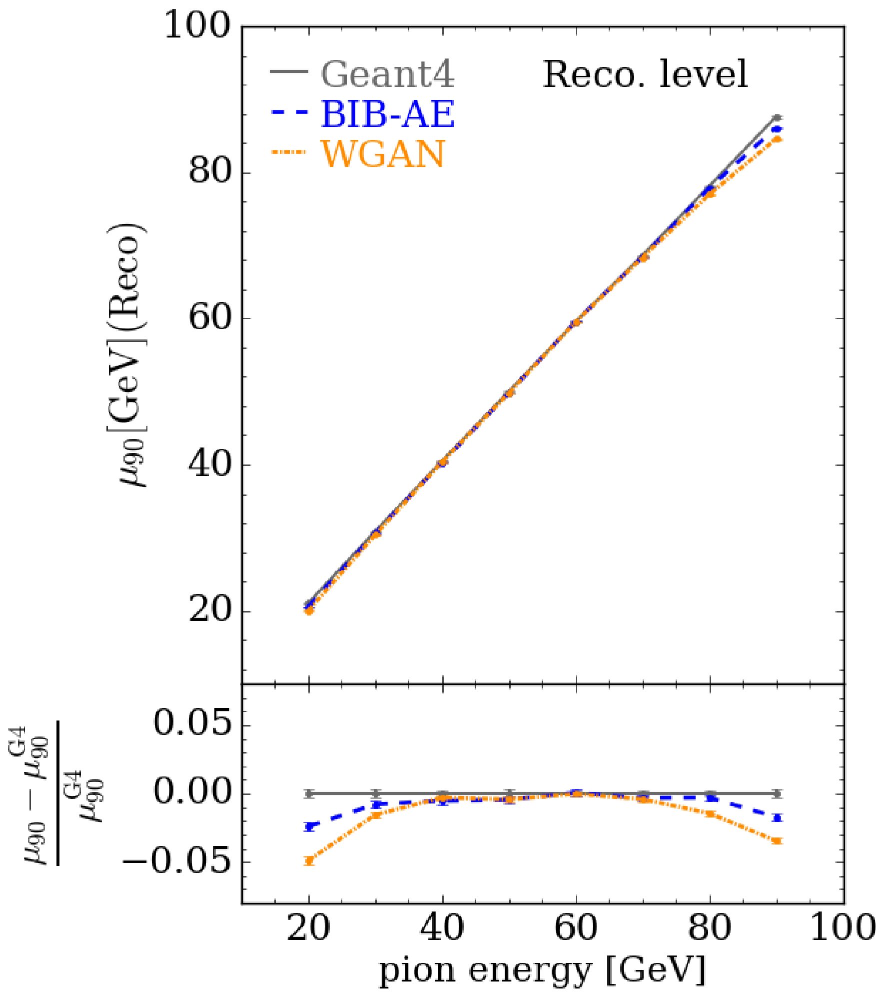
..with Generative Models

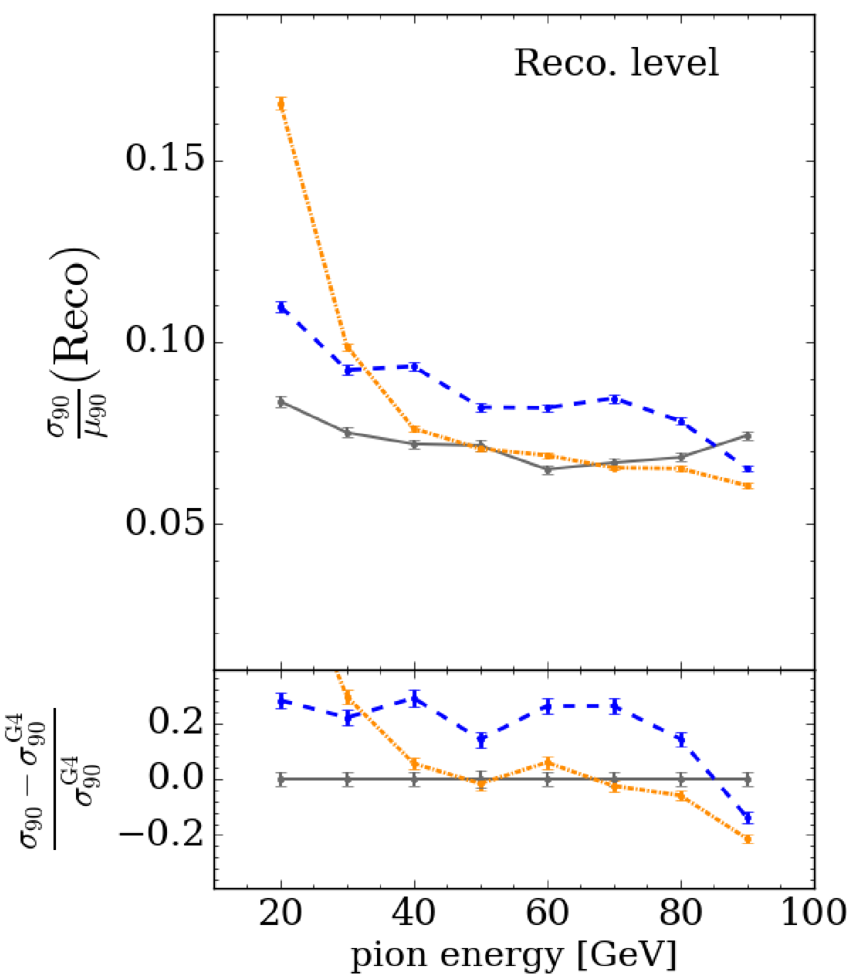




- First attempts to integrate generative ML models into the reconstruction workflow

Pion Showers after Reconstruction

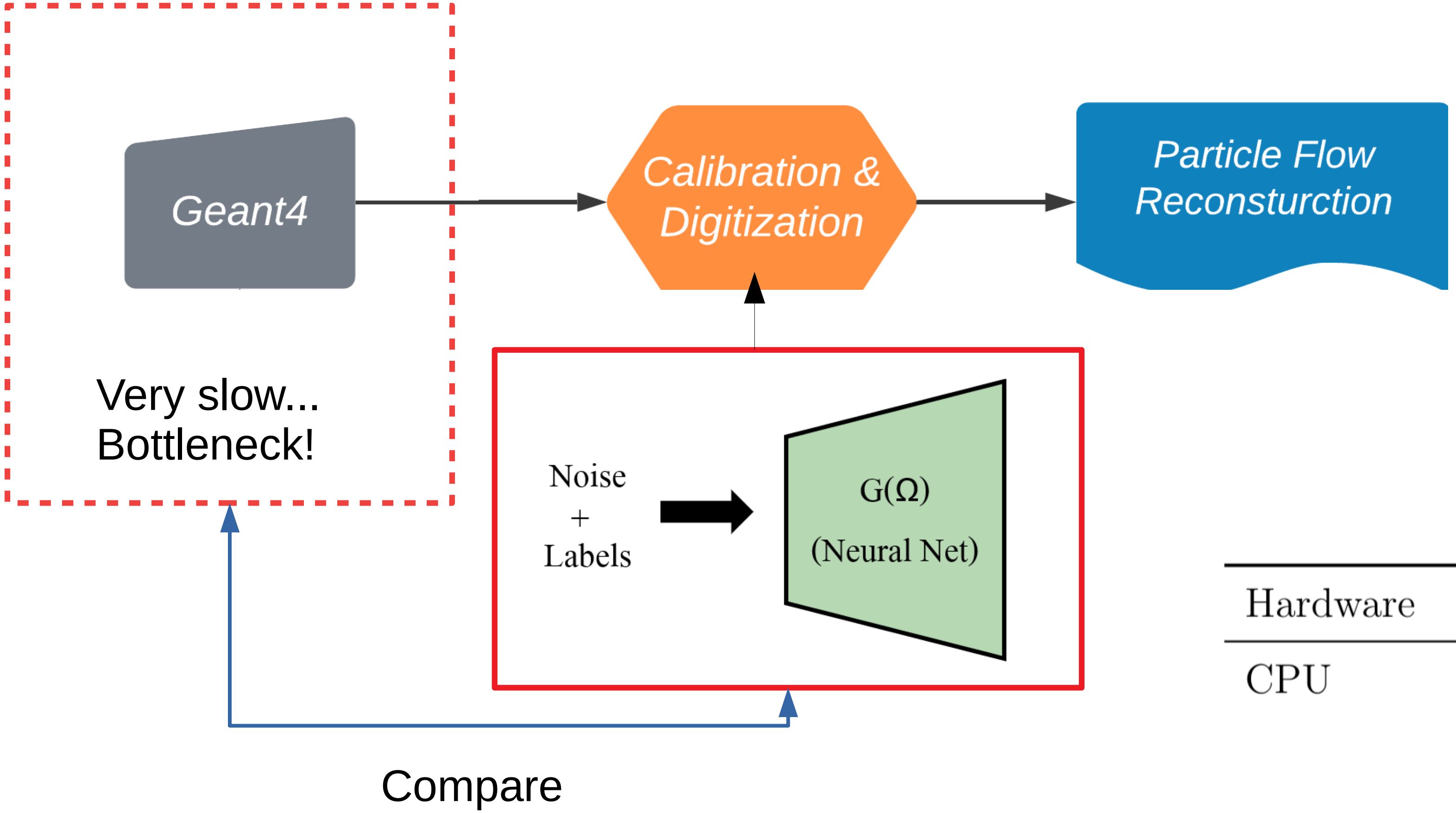


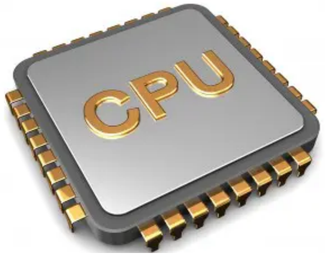


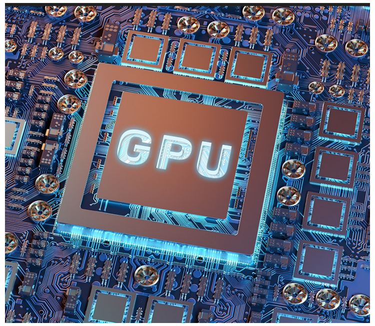
Both models show some discrepancy up to 3-5% at the edges.

Very good agreement by **WGAN** in the middle incident energies.

Generation Time







Hardware	Simulator	Time / Shower [ms]	Speed-up
CPU	GEANT4	2684 ± 125	$\times 1$
	WGAN	47.923 ± 0.089	$\times 56$
	BIB-AE	350.824 ± 0.574	$\times 8$
GPU	WGAN	0.264 ± 0.002	$\times 10167$
	BIB-AE	2.051 ± 0.005	$\times 1309$

Both models offer significant speedups!

Conclusion

Achieved

- Generative models hold promise for fast simulation of calorimeter showers with high fidelity
- Demonstrated high fidelity simulation of hadronic showers with generative models
  - Submitted to *Machine Learning: Science and Technology*

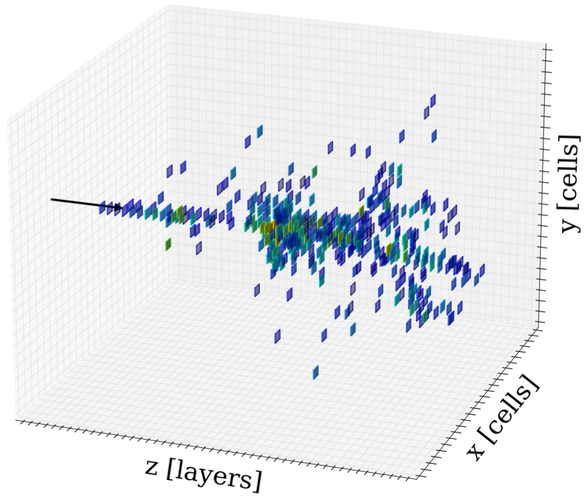
Ongoing Work

- Vary energy and angle simultaneously and study effect on performance
- Incorporate angular conditioning in more sophisticated architectures e.g. BIB-AE

Next Steps

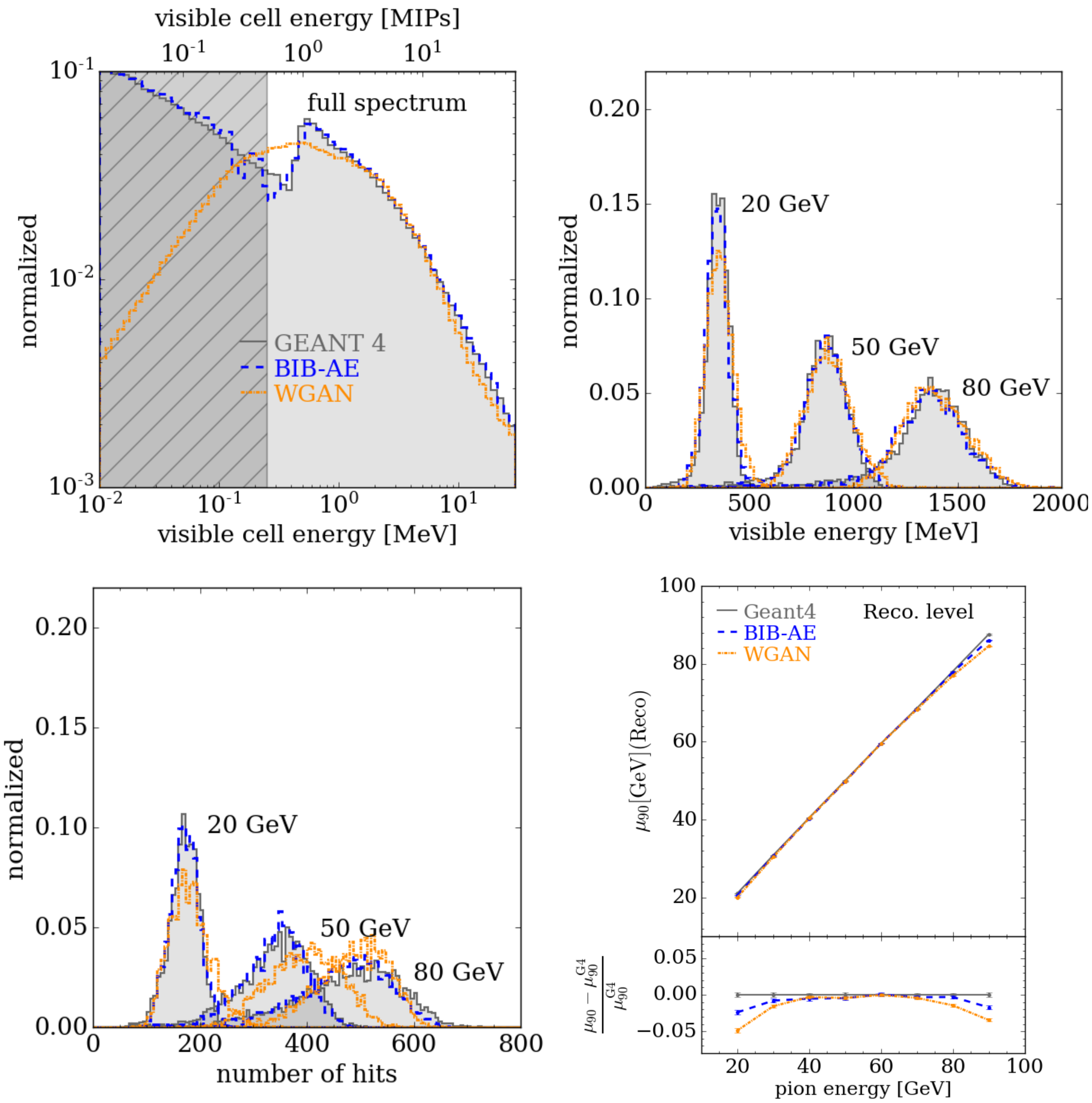
- Simulation of hadronic showers including HCAL and ECAL

generated shower by BIB-AE



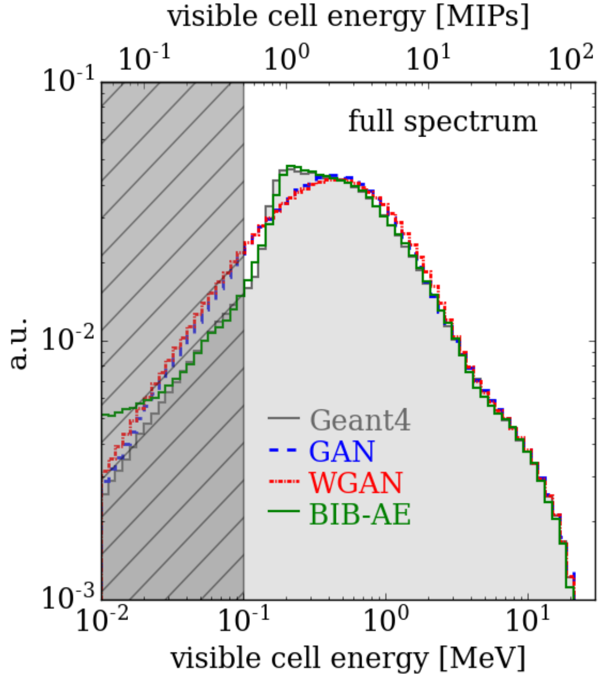
arXiv:2112.09709

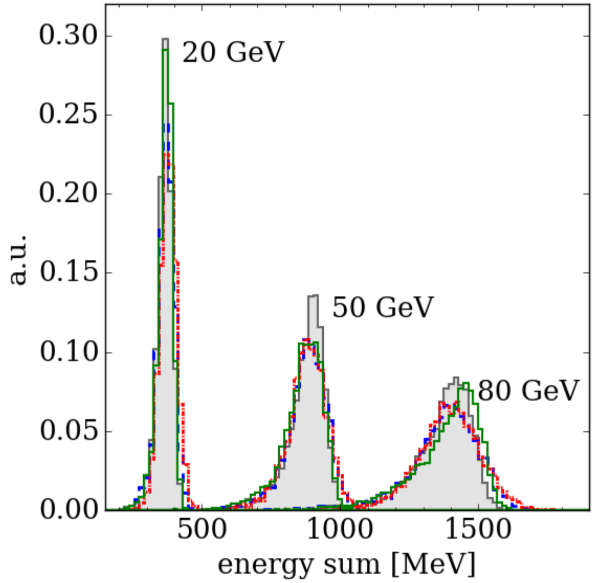
Backup

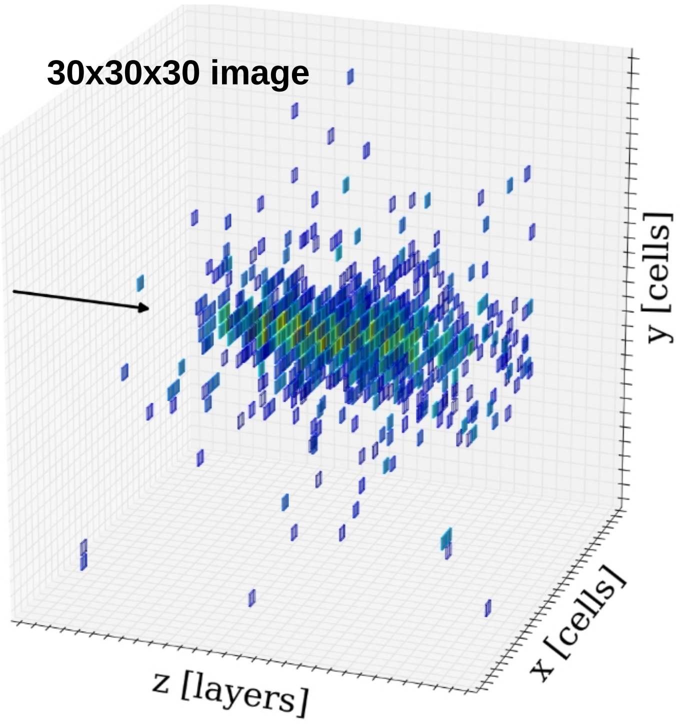


visible cell energy [MIPs]
full spectrum
GEANT 4
BIB-AE
WGAN
normalized
visible cell energy [MeV]
20 GeV
50 GeV
80 GeV
normalized
visible energy [MeV]
20 GeV
50 GeV
80 GeV
normalized
number of hits
Geant4
BIB-AE
WGAN
Reco. level
μ_{90}[GeV](Reco)
$\frac{\mu_{90}-\mu_{90}^{G4}}{\mu_{90}^{G4}}$
pion energy [GeV]

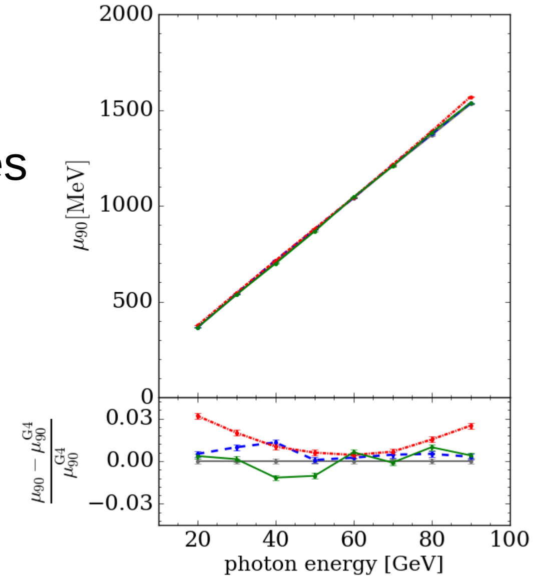
Photon Showers







High fidelity of shower properties are achieved

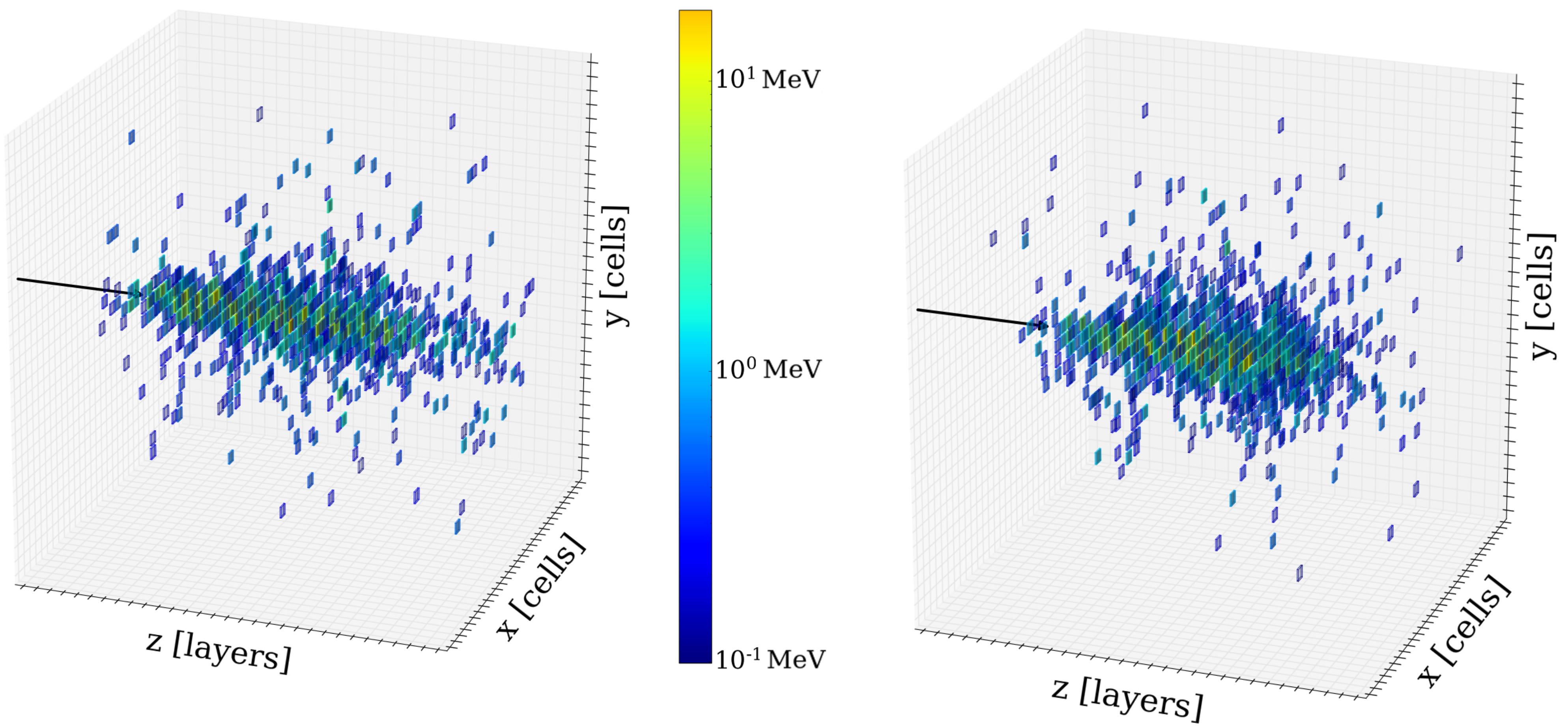


Hardware	Simulator	Photons	
		Time/shower[ms]	Speed-up
CPU	Geant4	4082±170	×1
	WGAN	61.44±0.03	×66
	BIB-AE	95.98±0.08	×43
GPU	WGAN	3.93±0.03	×1039
	BIB-AE	1.60±0.03	×2551

Significant speed ups

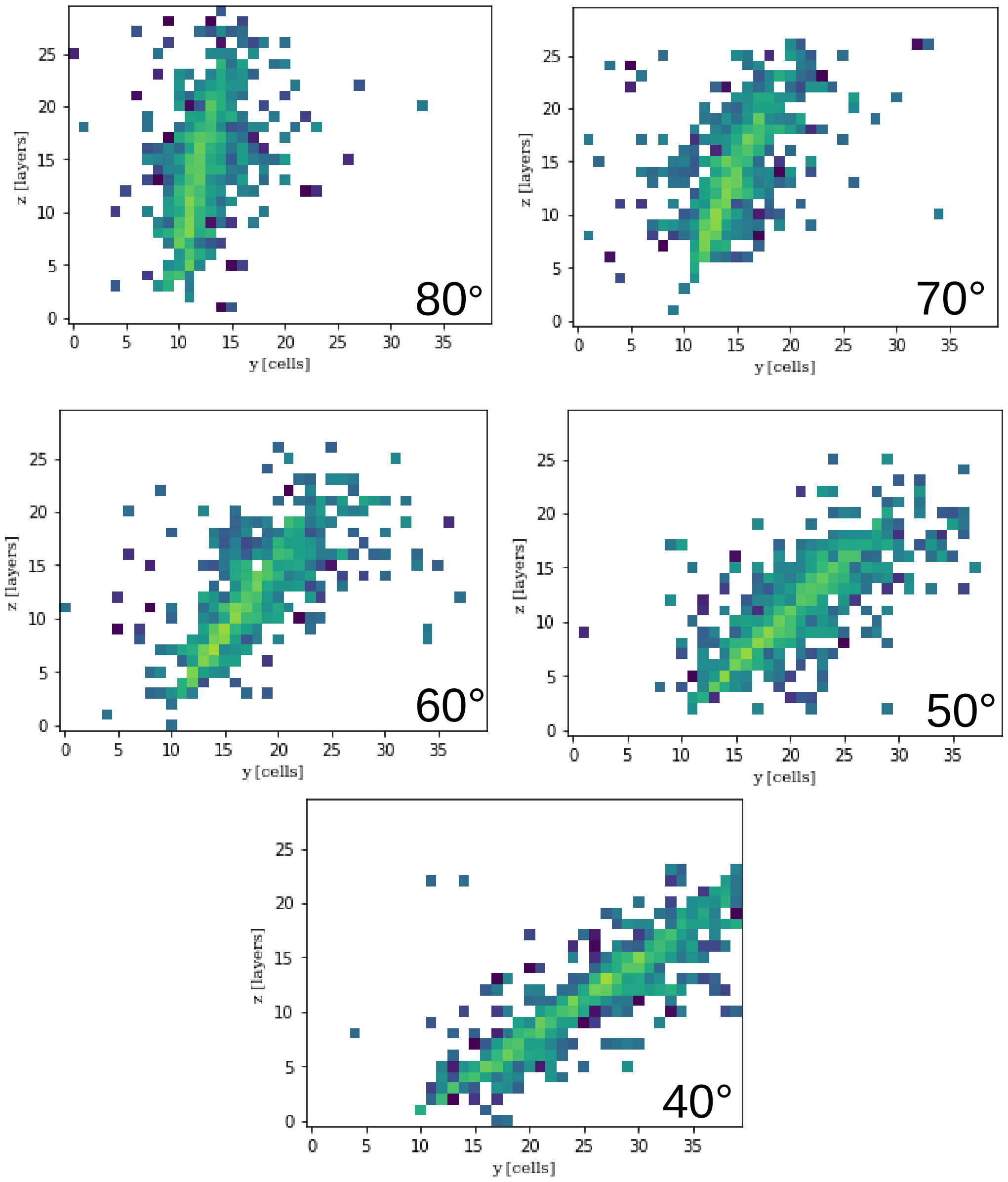
Buhmann, et al.: **Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed.** Comput Softw Big Sci 5, 13 (2021)

Photon Showers

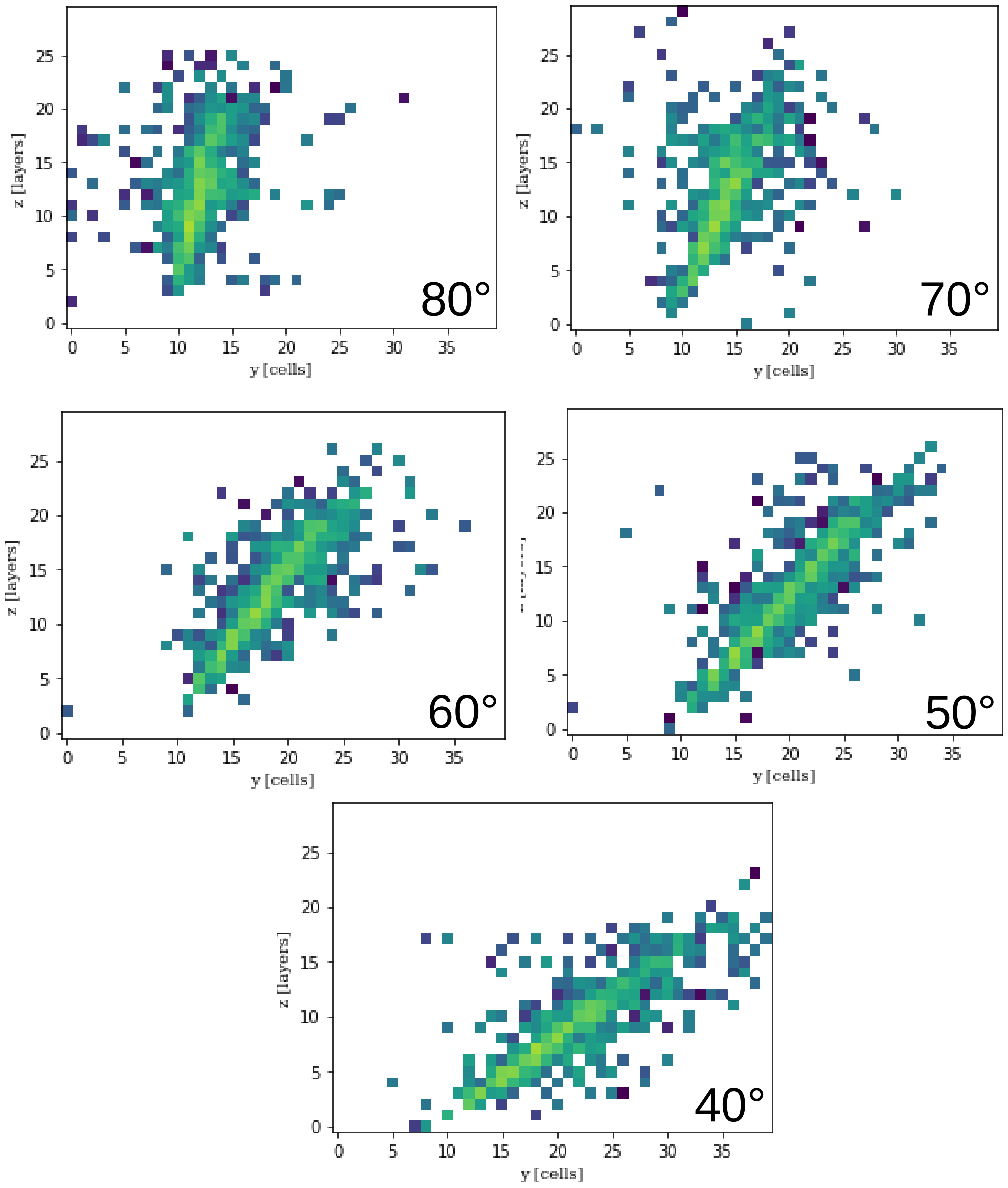


Ongoing work: Add angular conditioning (preliminary)

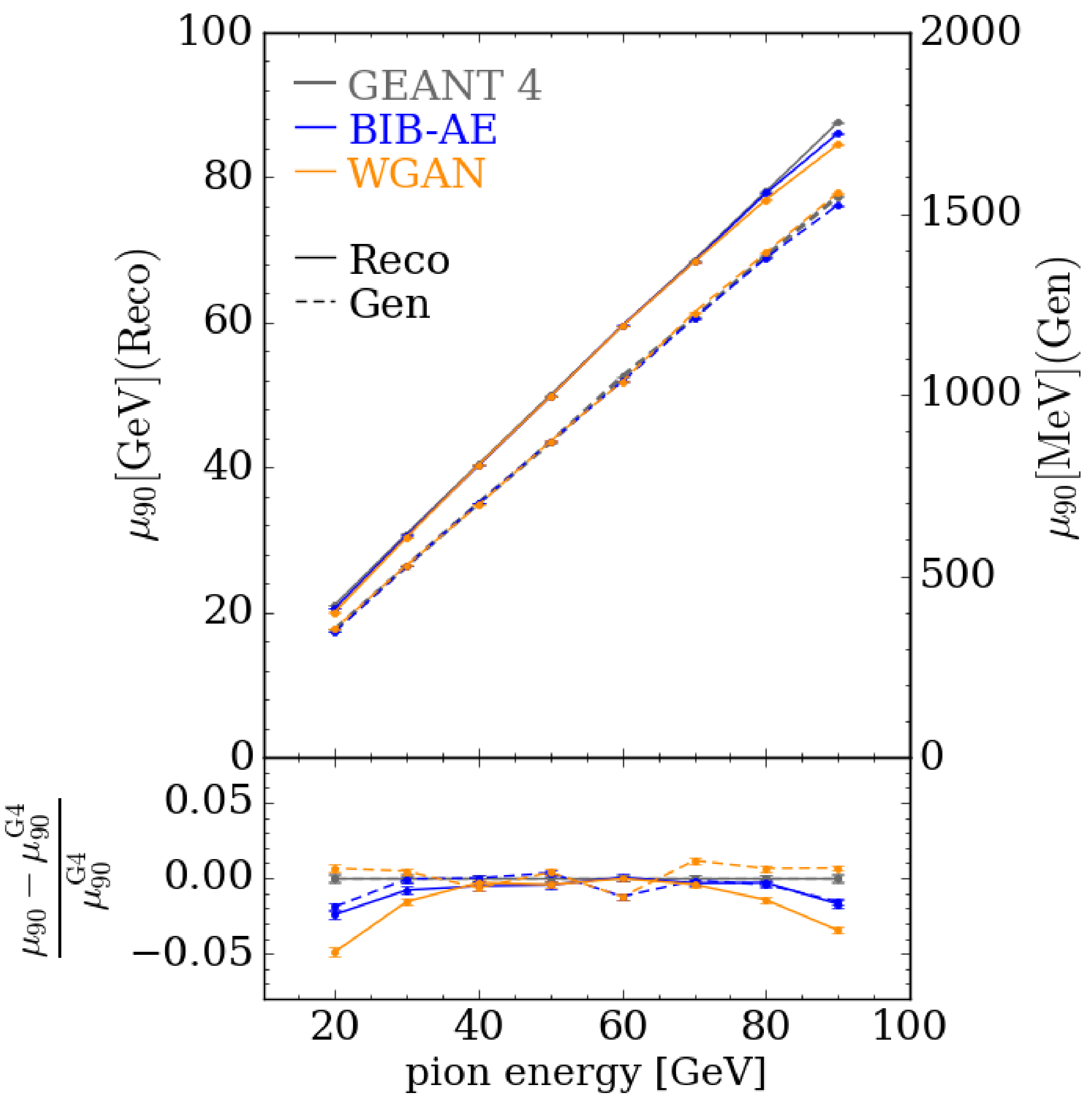
GEANT4

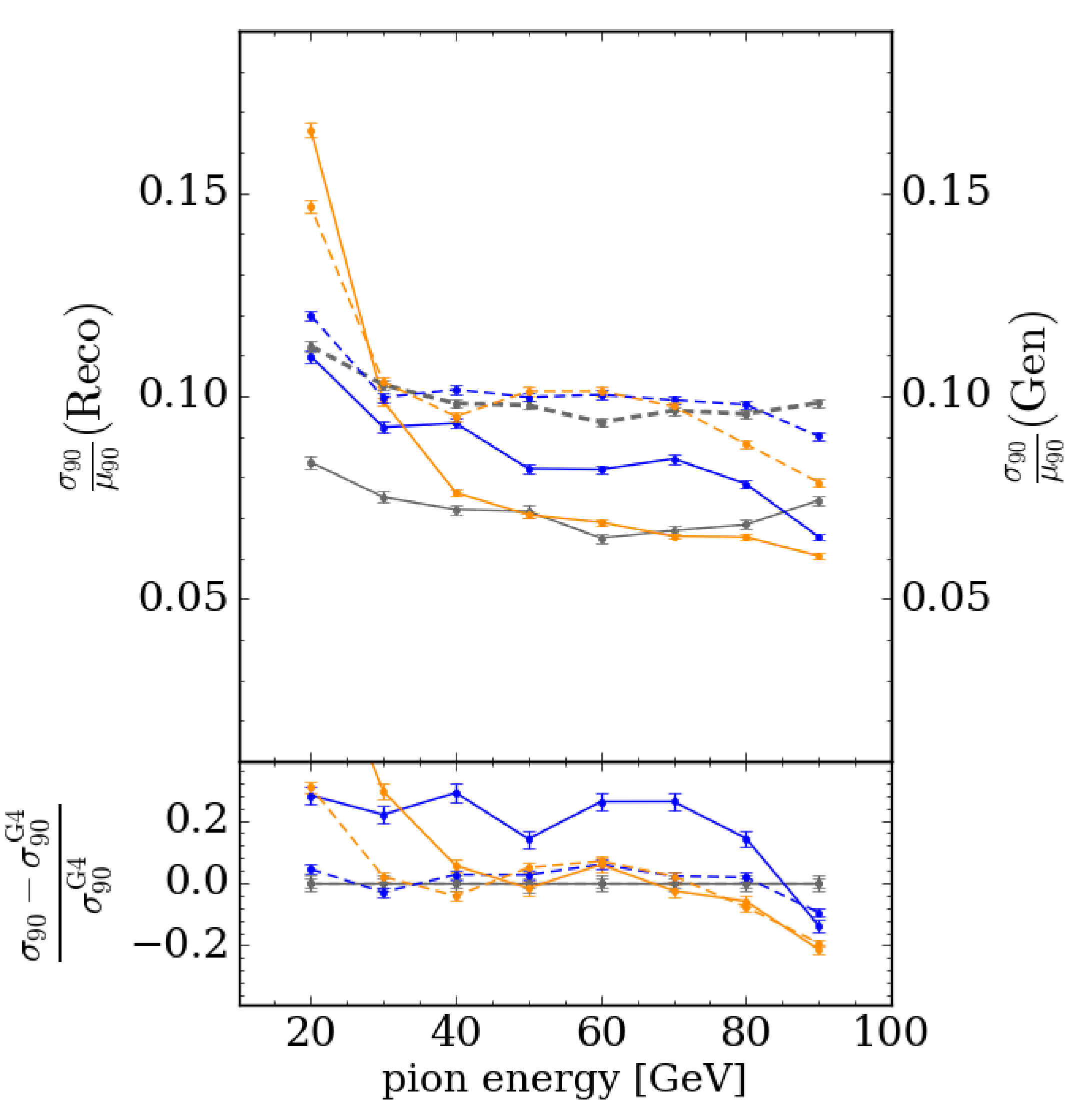


GAN



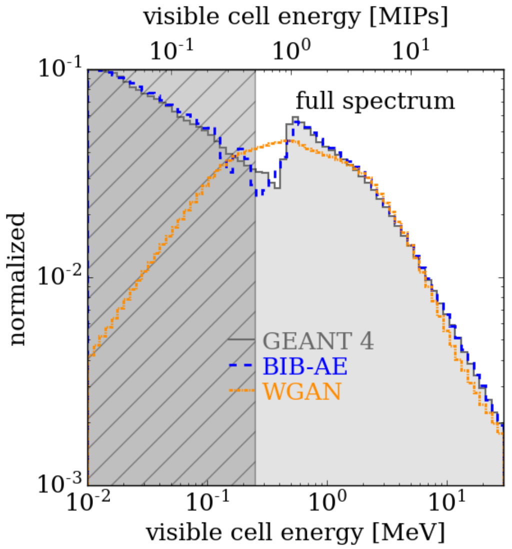
Pion Showers: Linearity and Resolution

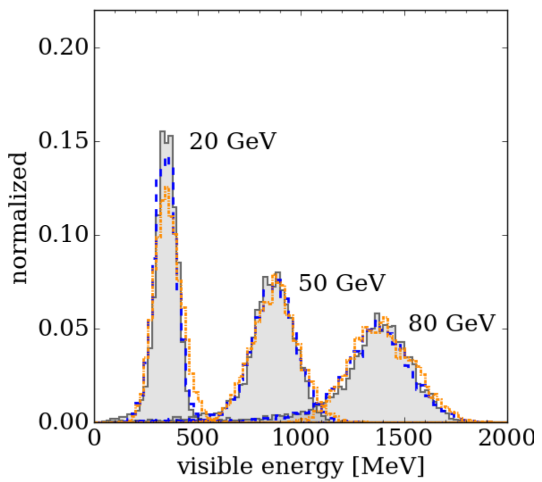


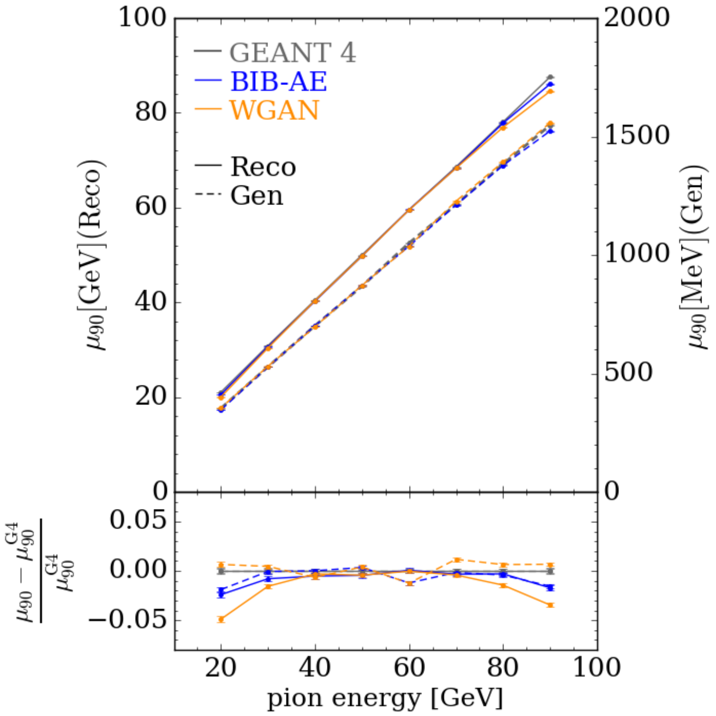


Pion Showers: Results

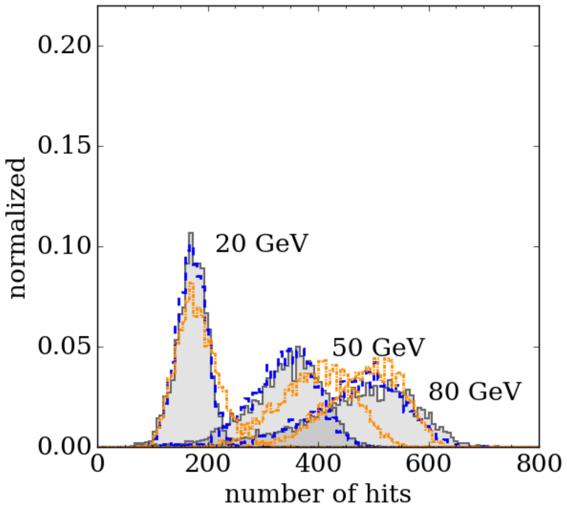
accepted to ML4PS workshop (NeurIPS 2021)

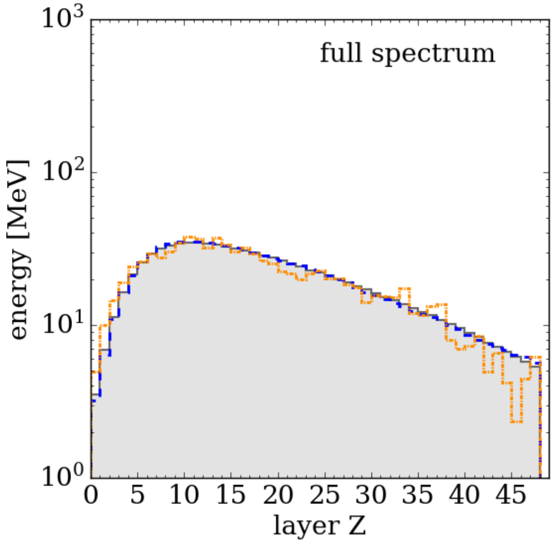






Overall good physics performance..





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GPU	WGAN	0.264 ± 0.002	×10167
	BIB-AE	2.051 ± 0.005	×1309

Both models offer significant speedups!

Pion Showers: Computing Time for Inference

Hardware	Simulator	Time / Shower [ms]	Speed-up
CPU	GEANT4	2684 ± 125	$\times 1$
	WGAN	47.923 ± 0.089	$\times 56$
	BIB-AE	350.824 ± 0.574	$\times 8$
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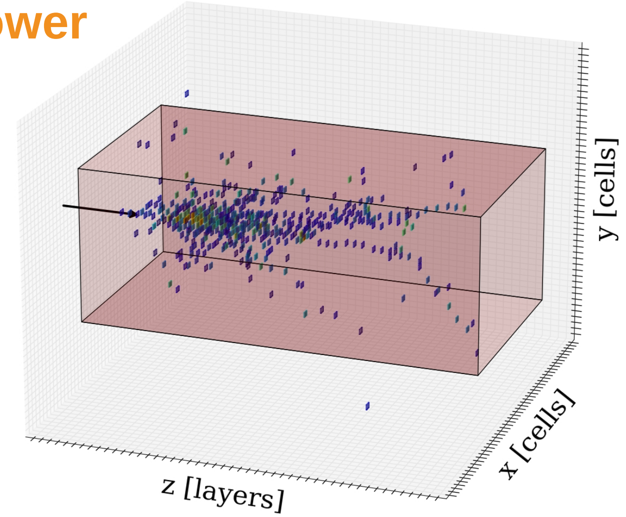
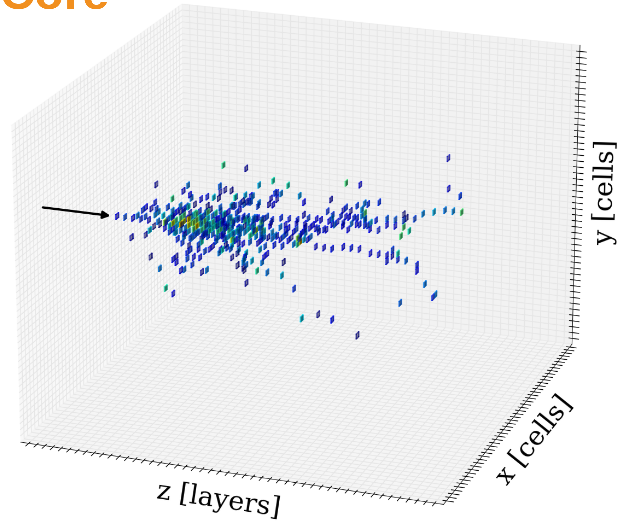
Speed-up of as much as four orders of magnitude on single core of Intel® Xeon® CPU E5-2640 v4 and NVIDIA® A100 for batch size 10000

Pion dataset

Full Shower



Shower Core



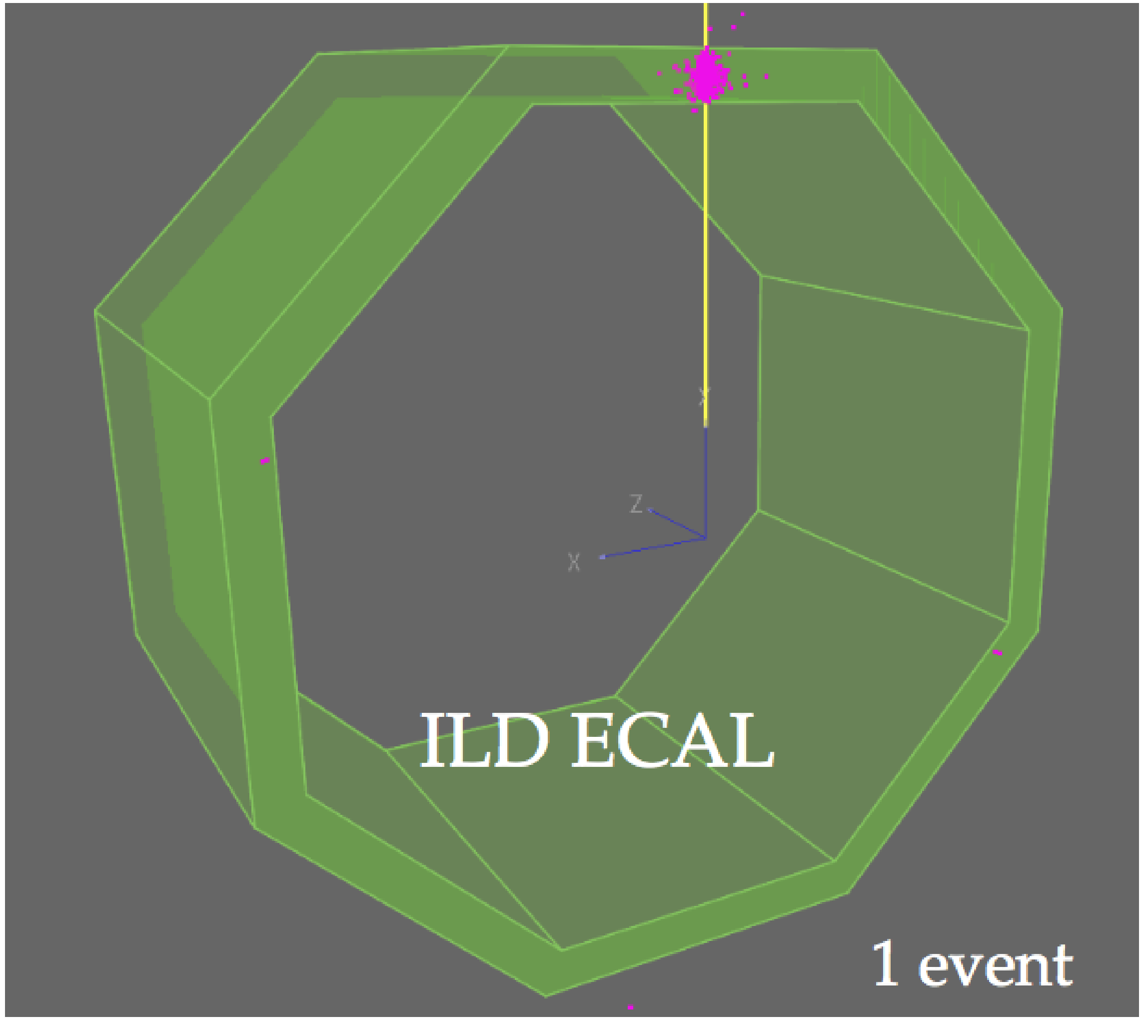
- AHCAL Option
- Remove ECal from geometry

- Significant sparsity in data
  - Use shower core
  - Barely lose any hits

- 500k showers
- Fixed incident point and angle
- Irregular geometry projected into 25x25x48 regular grid
- Uniform energy: 10-100 GeV

Conditioning requirements for a general simulation

- Conditioning for a general calorimeter simulation:
  - Energy ✓
  - Incidence point
  - Two angles
    - Polar angle: θ
    - Azimuthal angle: ϕ



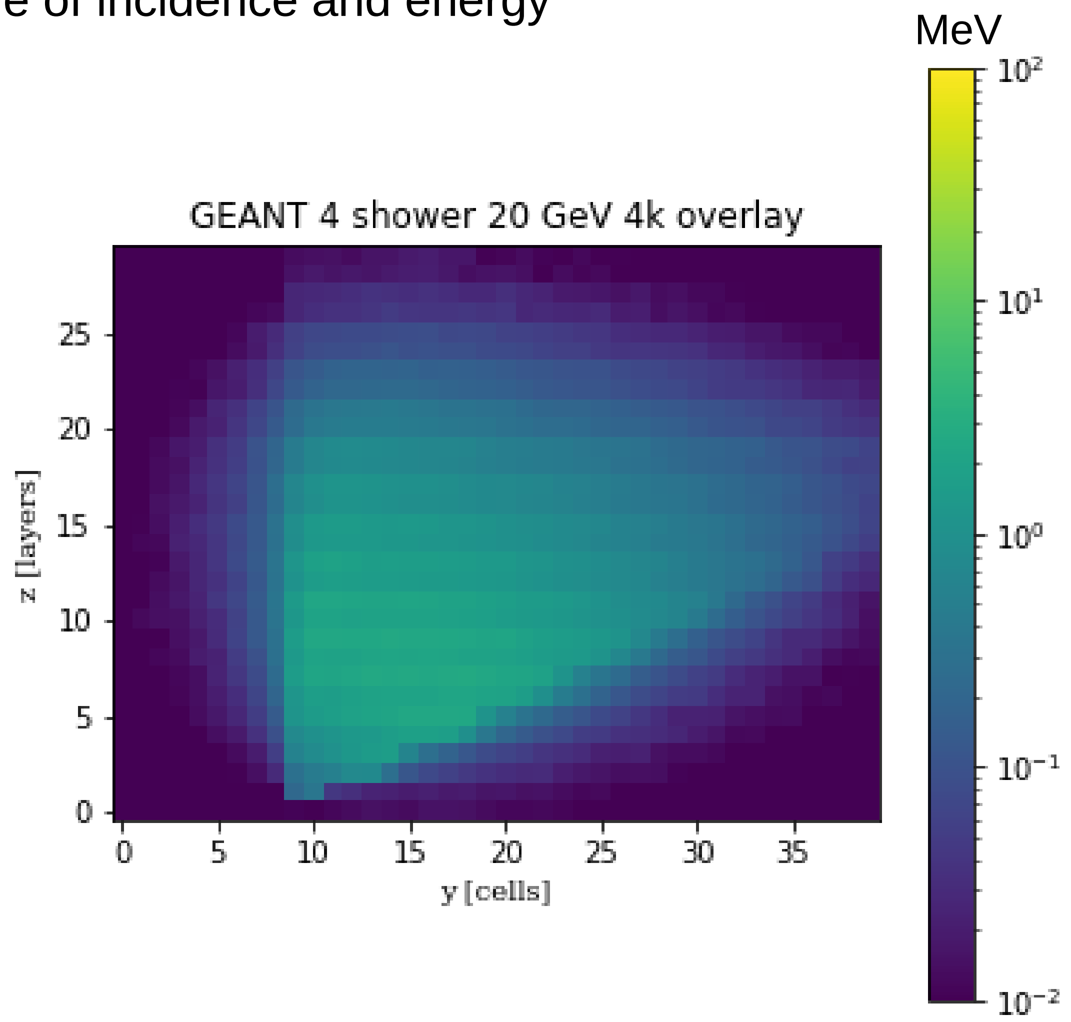
Angular conditioning- Training data

- In Progress: condition generative networks on particle's angle of incidence and energy

- Start simple:
  - Fixed energy- 20 GeV
  - Only vary polar angle in one direction- from 90°-30°
  - Fixed particle type- photons

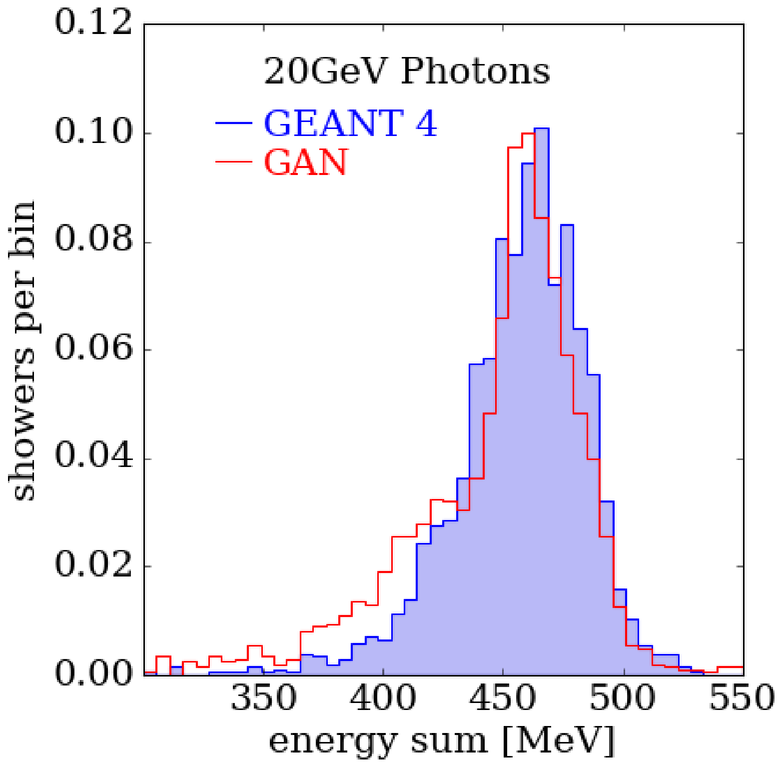
- Problem: How to make sure the full shower is contained?
  - Extend the selected grid in y: shape (30,30,40) (z,x,y)
  - Shift gun position

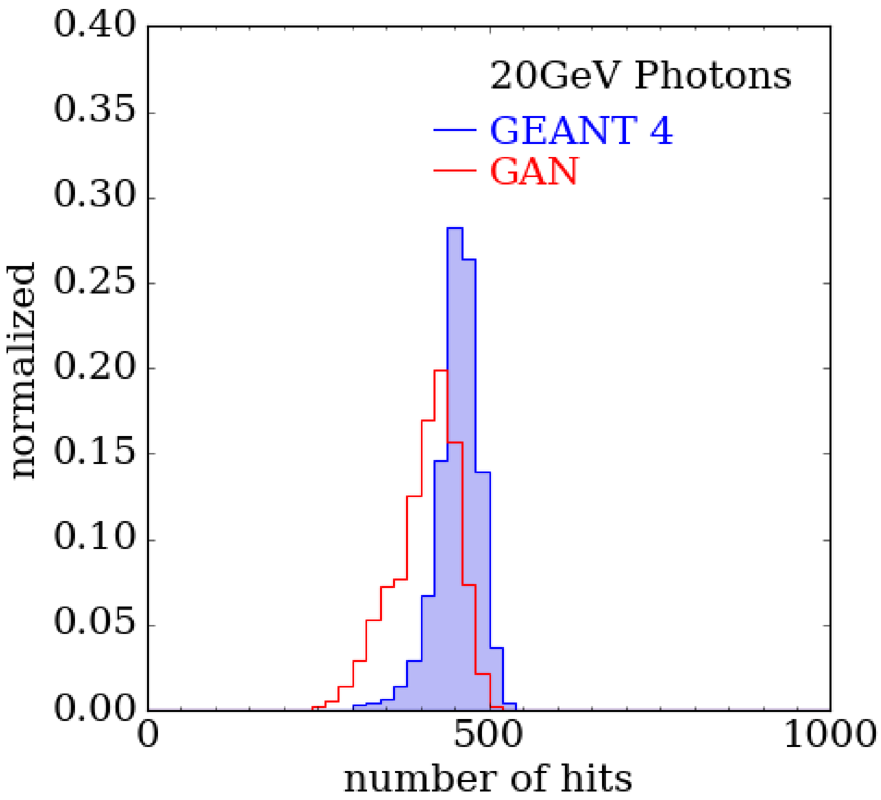
- Using 132k showers for training

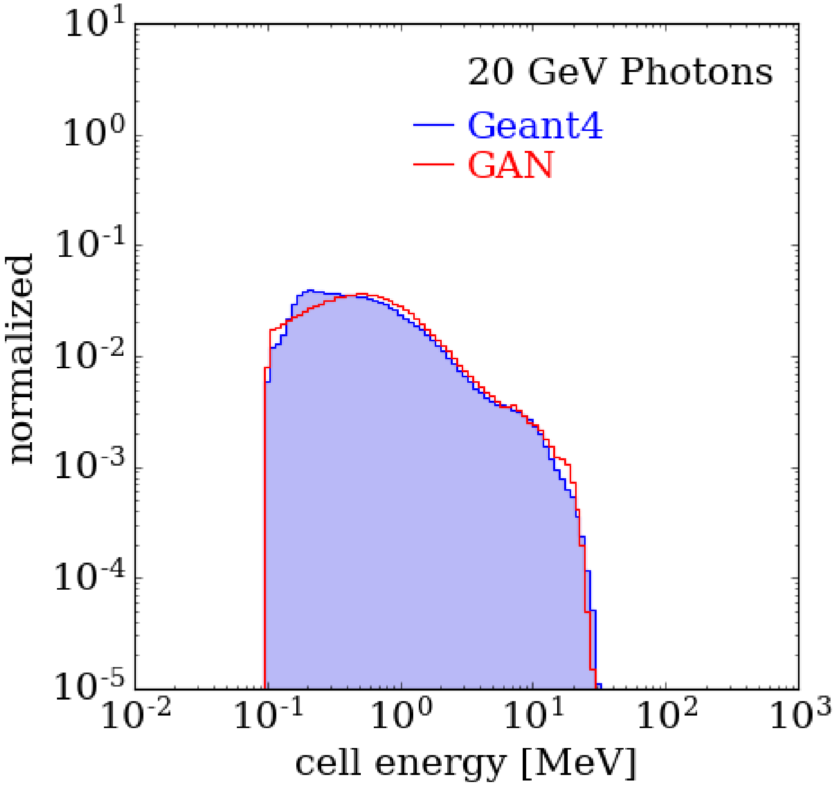


Angular conditioning- Some physics distributions

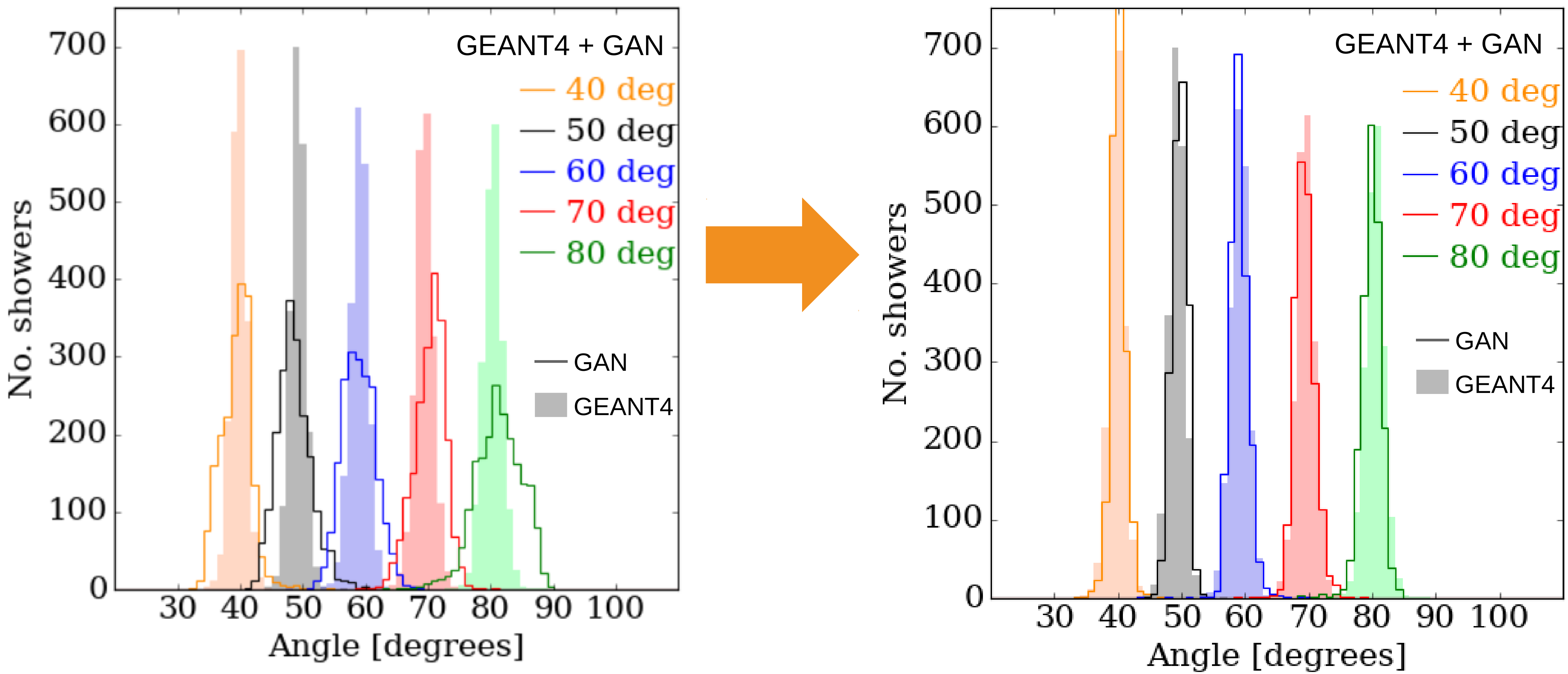
- Compare generated and GEANT4 distributions for a fixed angle of 60 degrees





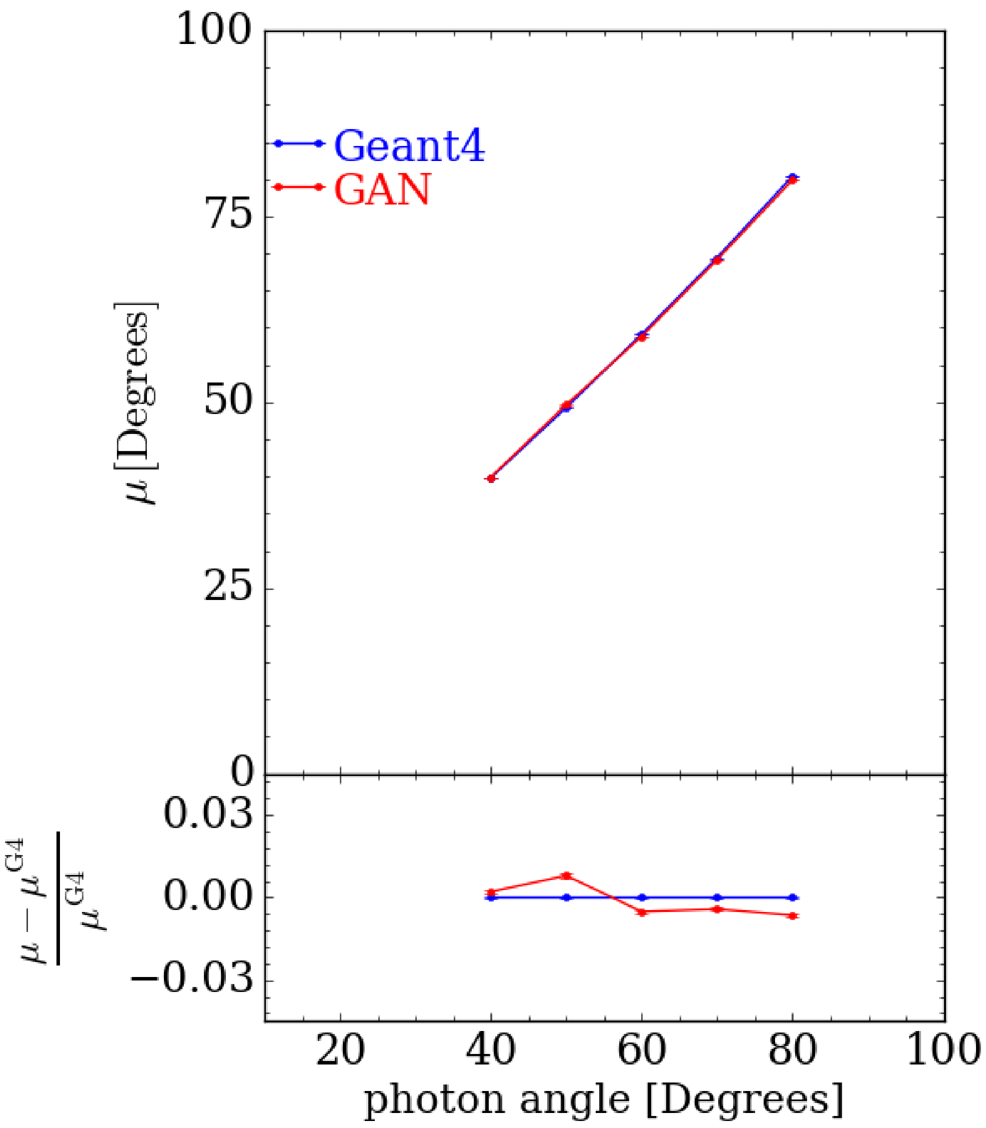


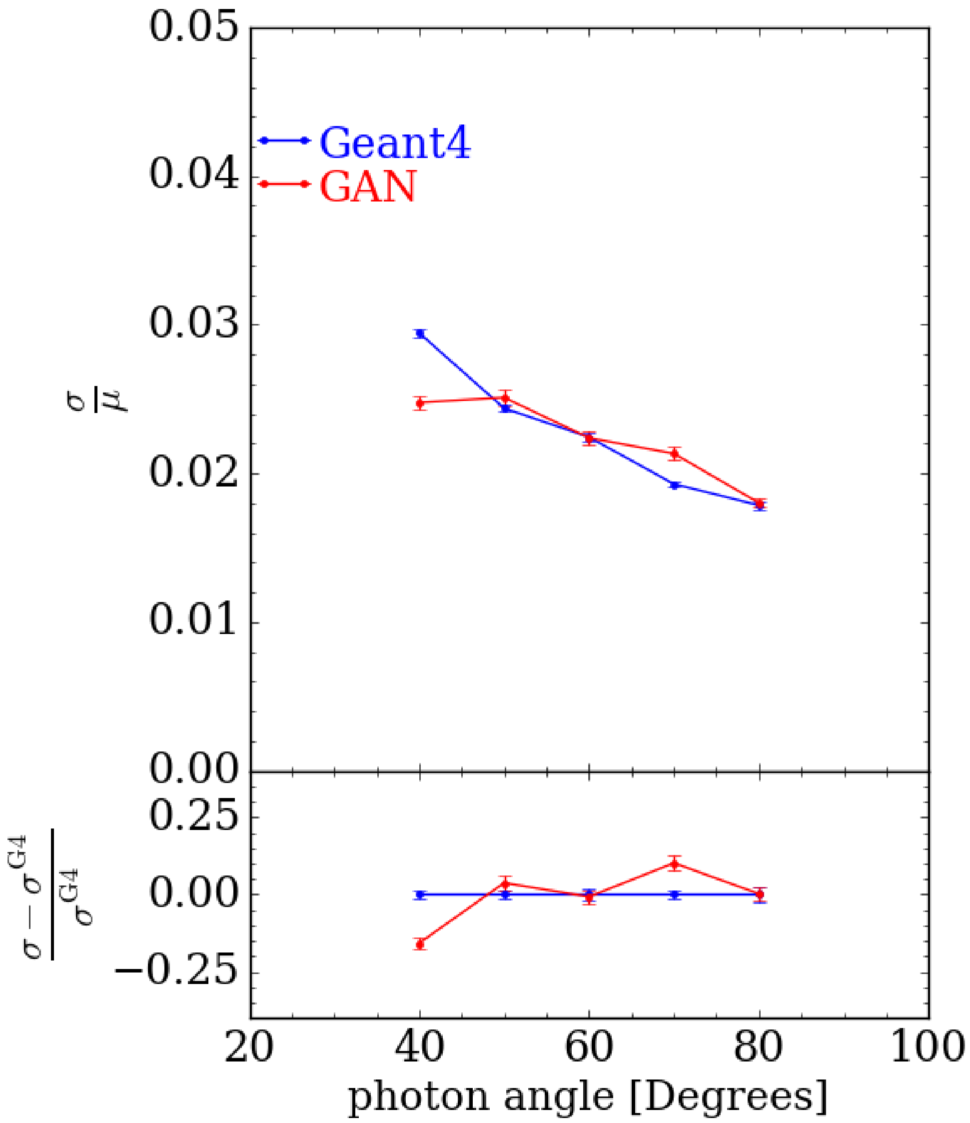
Angular conditioning- With a Constrainer Network



Angular linearity and resolution

- Good overall agreement



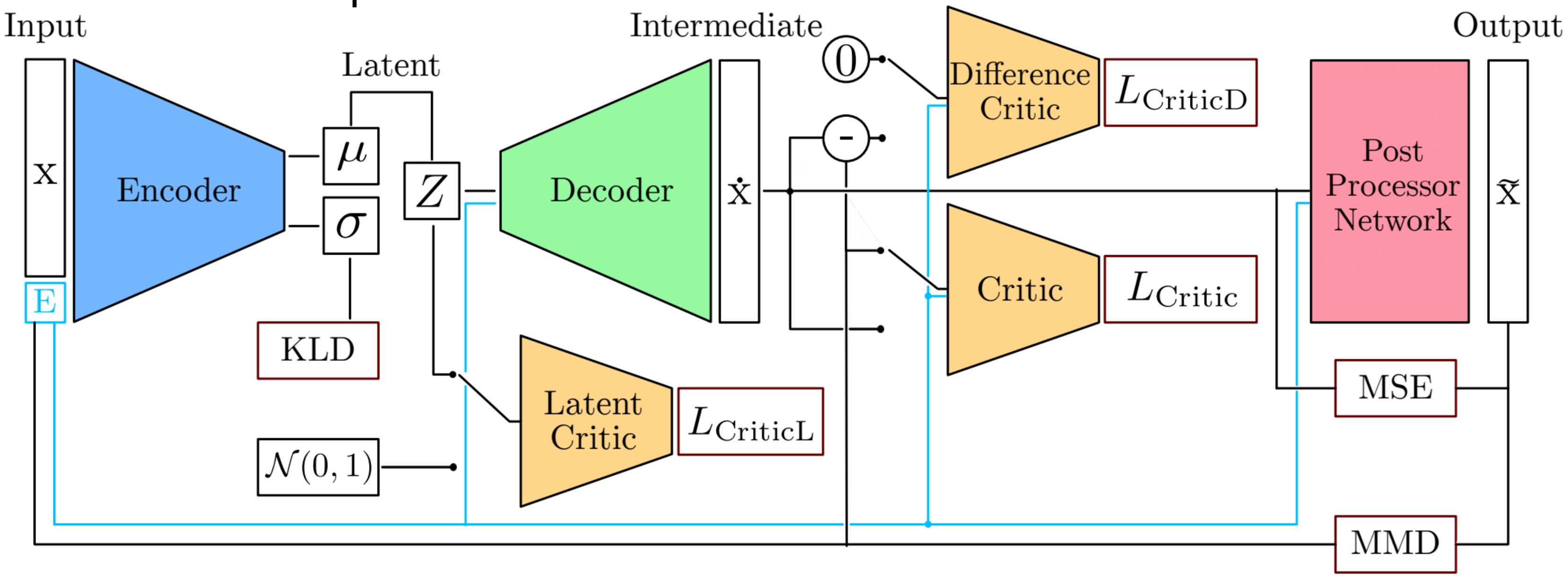


Architectures: BIB-AE

More Details

- Unifies features of both GANs and VAEs
- Adversarial critic networks rather than pixel-wise difference a la VAEs
- Improved latent regularisation: additional critic and MMD term
- Post-Processor network: Improve per-pixel energies; second training

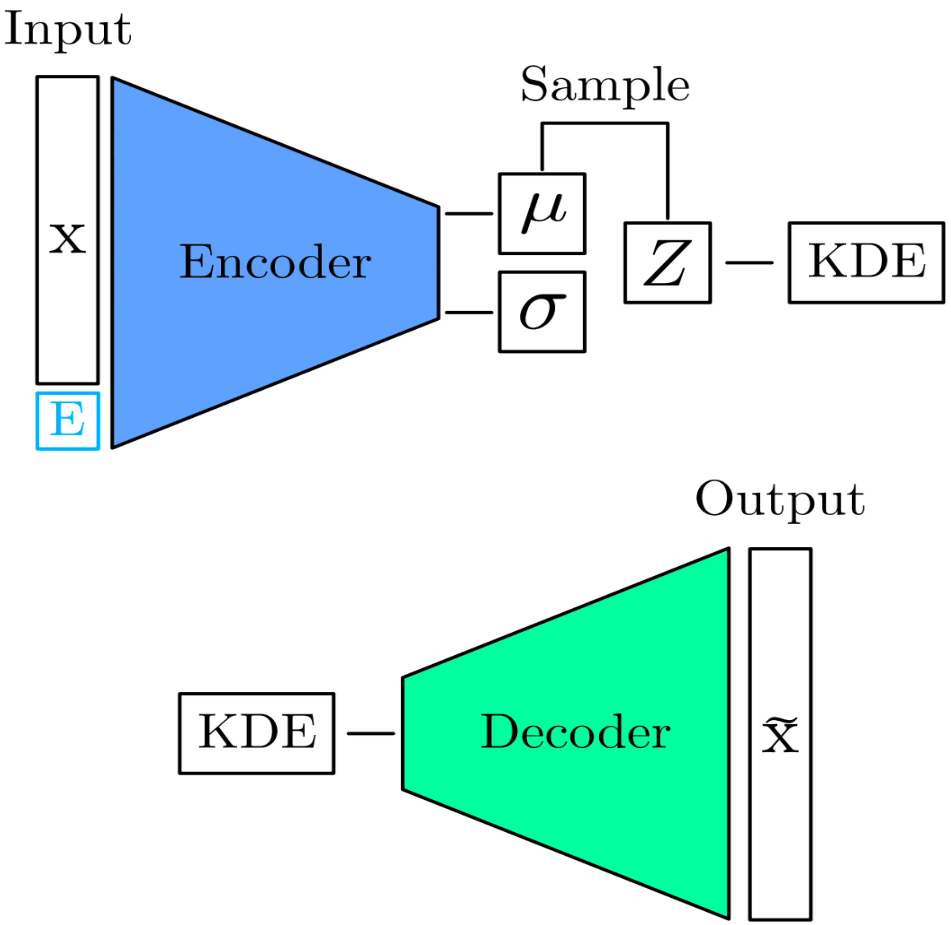
- Updates and improvements:
  - Dual and resetting critics: prevent artifacts caused by sparsity
  - Batch Statistics: prevent outliers/ mode collapse
  - Multi-dimensional KDE sampling: better modeling of latent space

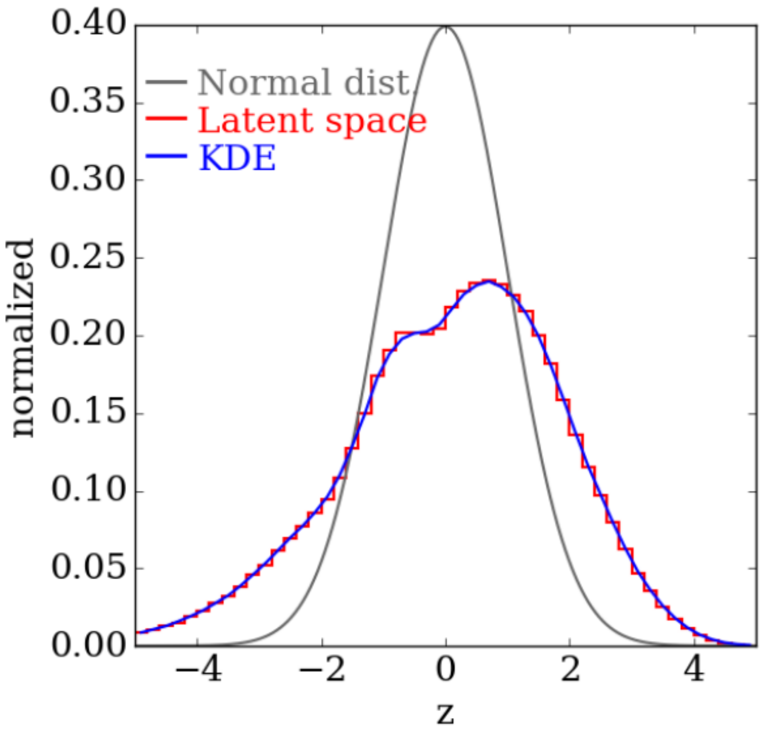


$$L_{\text{BIB-AE}} = \text{KLD} + L_{\text{CriticL}} + L_{\text{Critic}} + L_{\text{CriticD}}$$

$$L_{\text{Post}} = \text{MMD} + \text{MSE}$$

Kernel Density Estimation: BIB-AE





Buhmann et. al: **Decoding Photons: Physics in the Latent Space of a BIB-AE Generative Network**, EPJ Web of Conferences 251, 03003 (2021)

Pion correlations

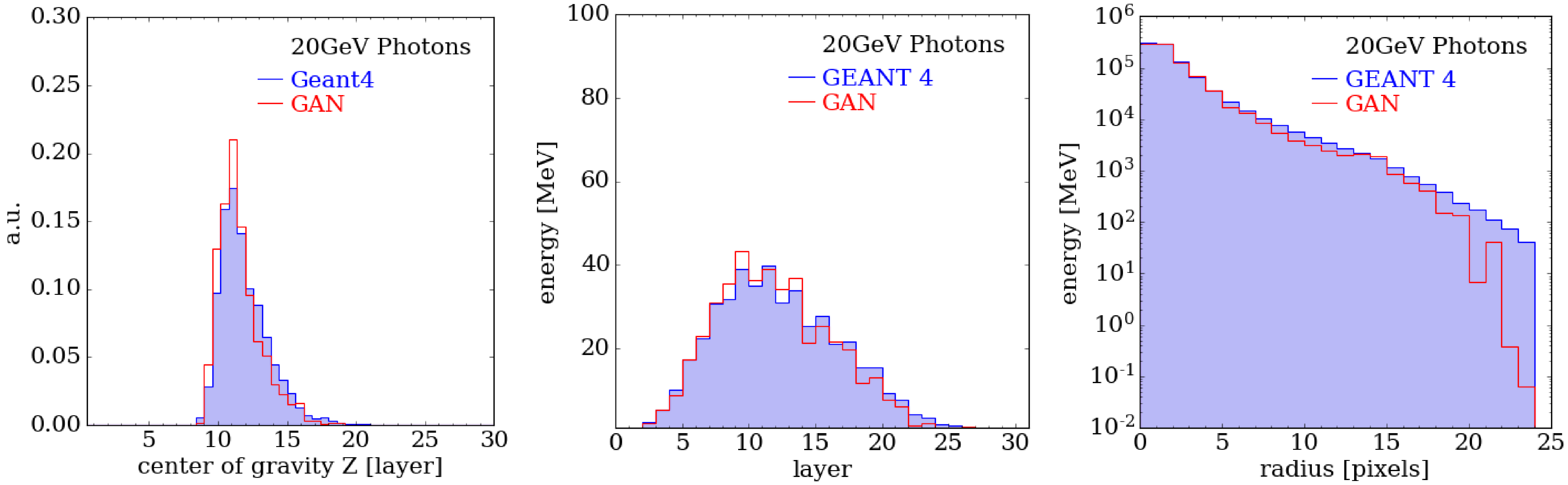
GEANT4 - BIB-AE

	$m_{1,x}$	$m_{1,y}$	$m_{1,z}$	$m_{2,x}$	$m_{2,y}$	$m_{2,z}$	E_{vis}	E_{inc}	n_{hit}	E_1/E_{vis}	E_2/E_{vis}	E_3/E_{vis}
$m_{1,x}$	0.00											
$m_{1,y}$	-0.00	0.00										
$m_{1,z}$	-0.01	-0.04	0.00									
$m_{2,x}$	-0.08	-0.00	-0.06	0.00								
$m_{2,y}$	-0.10	-0.03	-0.05	0.01	0.00							
$m_{2,z}$	-0.06	0.01	-0.06	-0.08	-0.05	0.00						
E_{vis}	0.03	-0.02	-0.01	0.09	0.09	0.06	0.00					
E_{inc}	0.01	-0.03	-0.00	0.08	0.09	0.06	-0.01	0.00				
n_{hit}	0.03	-0.02	-0.02	0.13	0.14	0.06	0.00	-0.01	0.00			
E_1/E_{vis}	0.00	0.03	0.00	0.04	0.04	0.04	0.01	0.00	0.02	0.00		
E_2/E_{vis}	-0.01	-0.00	-0.03	0.02	-0.02	0.01	-0.02	-0.02	-0.01	0.02	0.00	
E_3/E_{vis}	-0.01	-0.04	0.00	-0.07	-0.04	-0.07	0.00	0.01	-0.01	-0.00	-0.03	0.00

GEANT4 - WGAN

	$m_{1,x}$	$m_{1,y}$	$m_{1,z}$	$m_{2,x}$	$m_{2,y}$	$m_{2,z}$	E_{vis}	E_{inc}	n_{hit}	E_1/E_{vis}	E_2/E_{vis}	E_3/E_{vis}
$m_{1,x}$	0.00											
$m_{1,y}$	-0.21	0.00										
$m_{1,z}$	0.20	-0.10	0.00									
$m_{2,x}$	-0.14	-0.17	-0.20	0.00								
$m_{2,y}$	-0.20	-0.28	-0.21	-0.18	0.00							
$m_{2,z}$	-0.14	-0.24	-0.17	-0.20	-0.23	0.00						
E_{vis}	0.14	0.19	-0.21	0.11	0.18	0.06	0.00					
E_{inc}	0.11	0.17	-0.13	0.01	0.09	0.03	-0.03	0.00				
n_{hit}	0.10	0.07	-0.26	-0.02	0.05	-0.09	0.04	-0.00	0.00			
E_1/E_{vis}	-0.17	0.05	0.02	0.16	0.15	0.14	0.14	0.10	0.15	0.00		
E_2/E_{vis}	0.11	0.09	-0.28	-0.00	0.03	-0.01	-0.06	-0.12	-0.01	0.15	0.00	
E_3/E_{vis}	0.09	-0.22	0.03	-0.26	-0.29	-0.31	-0.15	-0.06	-0.27	0.03	-0.28	0.00

Angular conditioning- 60 degree shower shape distributions



Angular conditioning- 80 degree other distributions